

# *Principles of Micro- and Nanofabrication for Electronic and Photonic Devices*

## **Materials: Structures and Synthesis**

**Xing Sheng 盛兴**

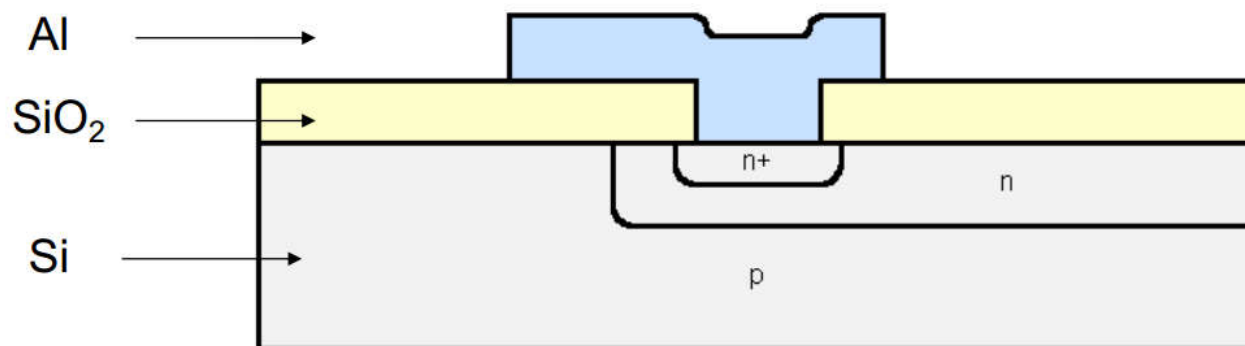


**Department of Electronic Engineering  
Tsinghua University**

**[xingsheng@tsinghua.edu.cn](mailto:xingsheng@tsinghua.edu.cn)**

# Raw Materials

## MOS: Metal-Oxide-Semiconductor



**Silicon**

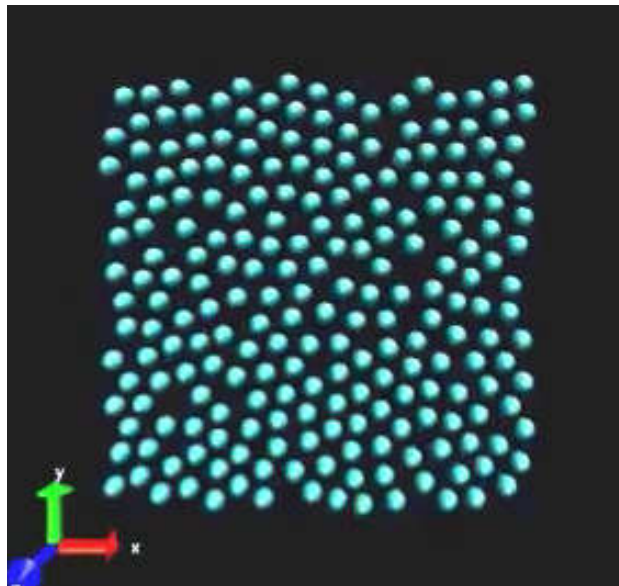
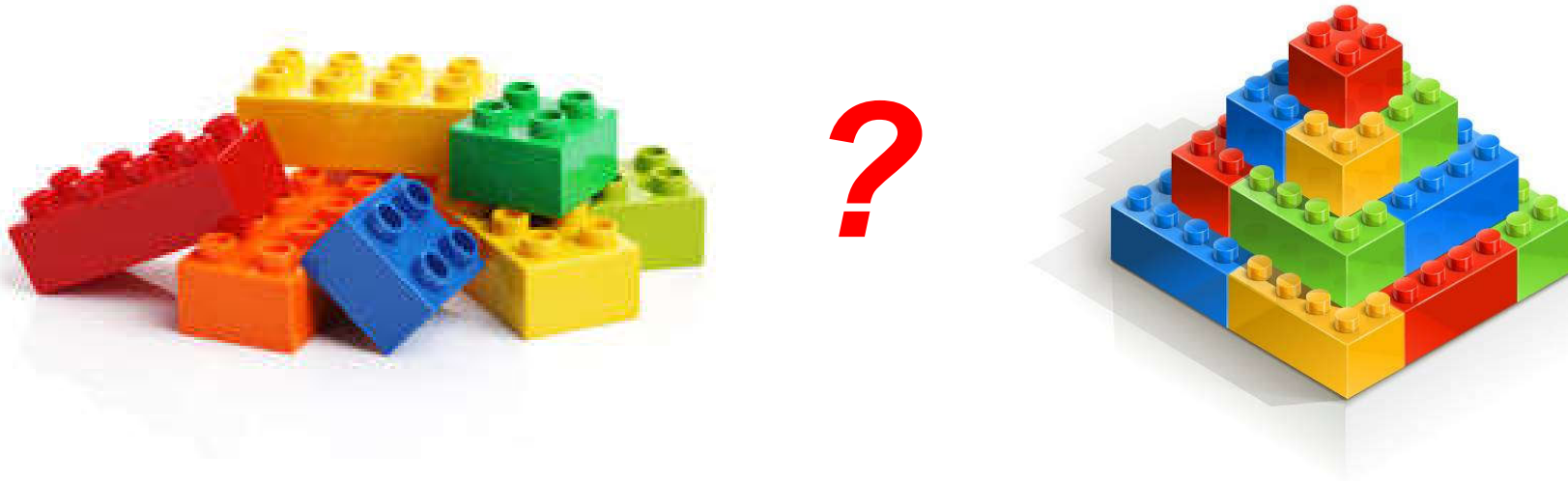


**SiO<sub>2</sub>**

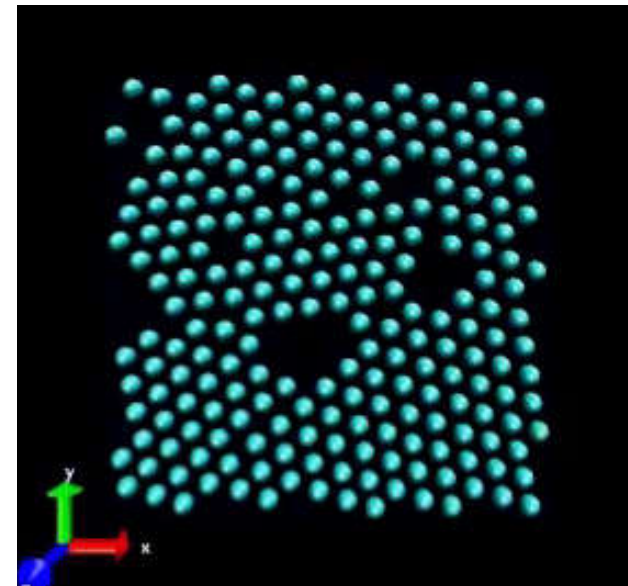


**Metal**

# Crystal Structures



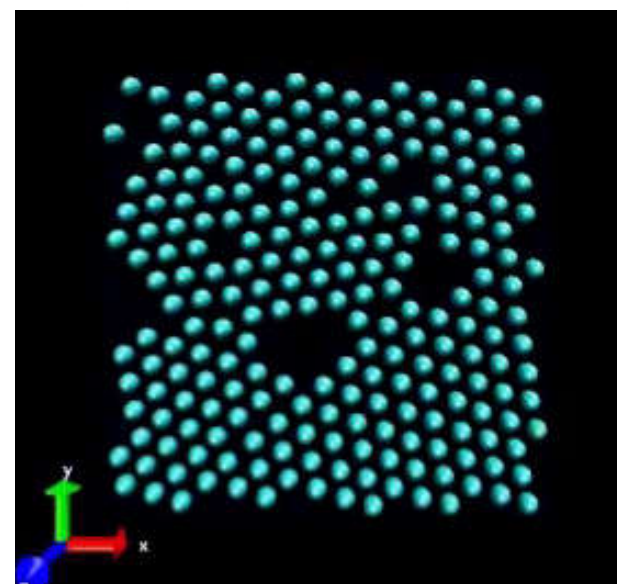
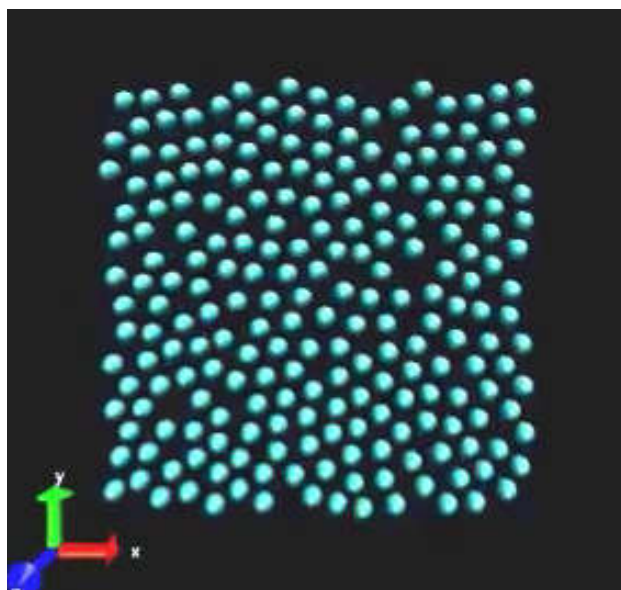
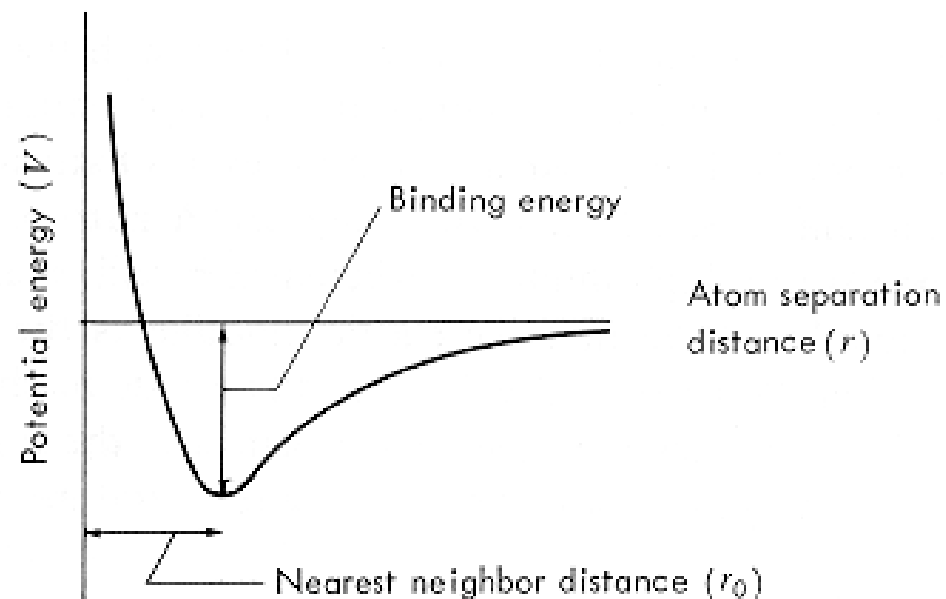
→  
Video



# It is all about *energy*

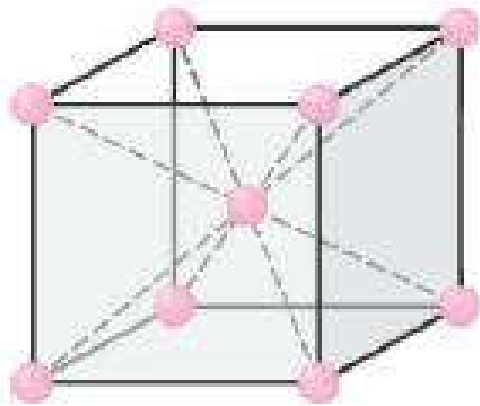
## Lennard-Jones Potential

$$V(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$



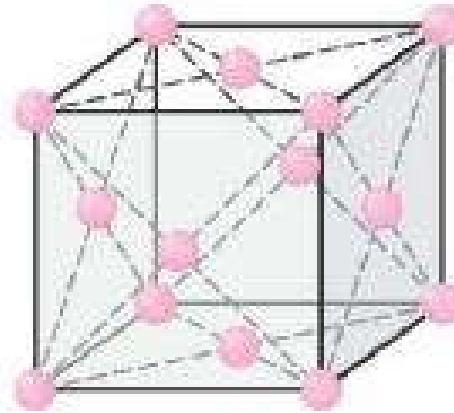
# Crystal Structures

Li, Na, Cr,...



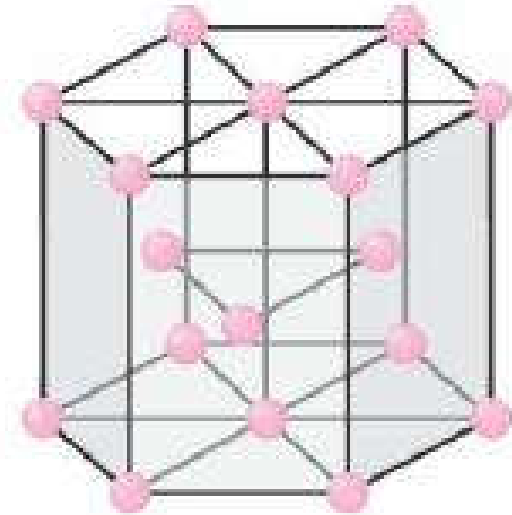
BCC

Al, Cu, Au,...



FCC

Mg, Zn, Ti,...



HCP

## ■ 3D:

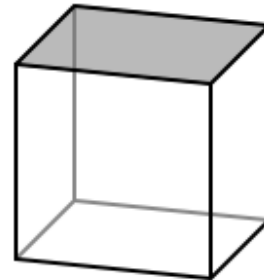
- 14 Bravais lattices
- 32 point groups
- 230 space groups

# Miller Indices

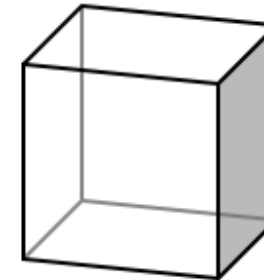
**$(lmn)$  plane**

**intercepts at**

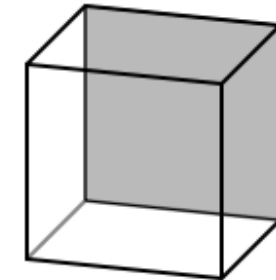
**$a_1/l, a_2/m, a_3/n$**



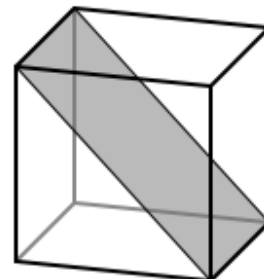
(001)



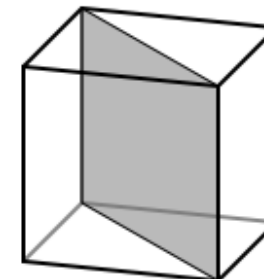
(100)



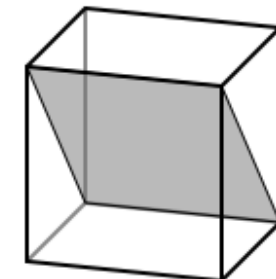
(010)



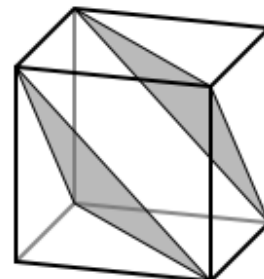
(101)



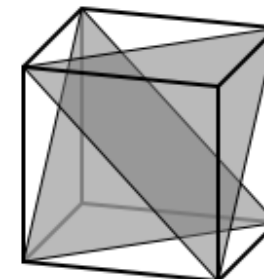
(110)



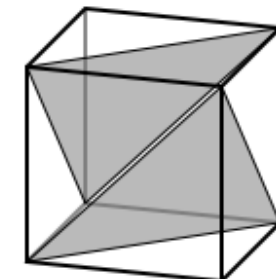
(011)



(111)



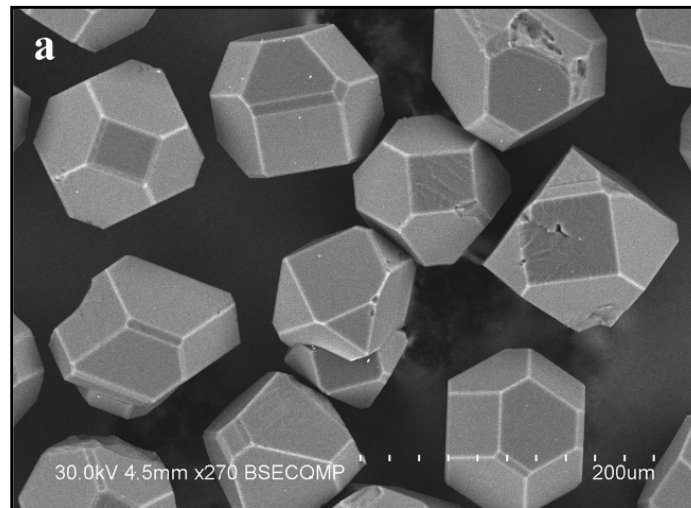
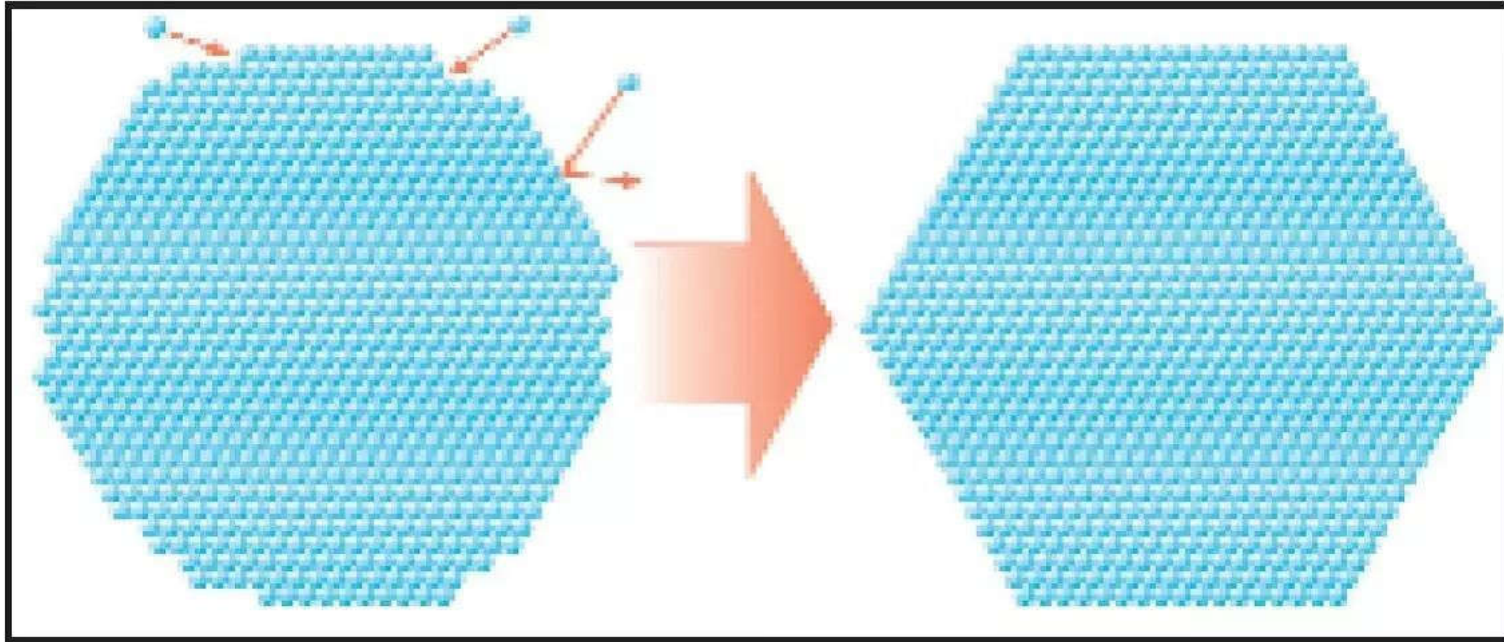
(11̄1)



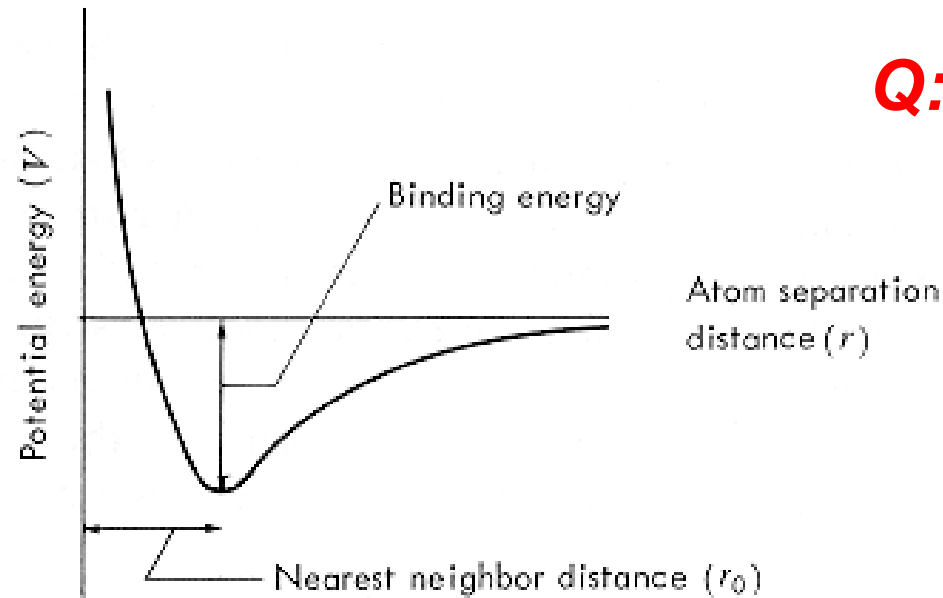
(1̄11)



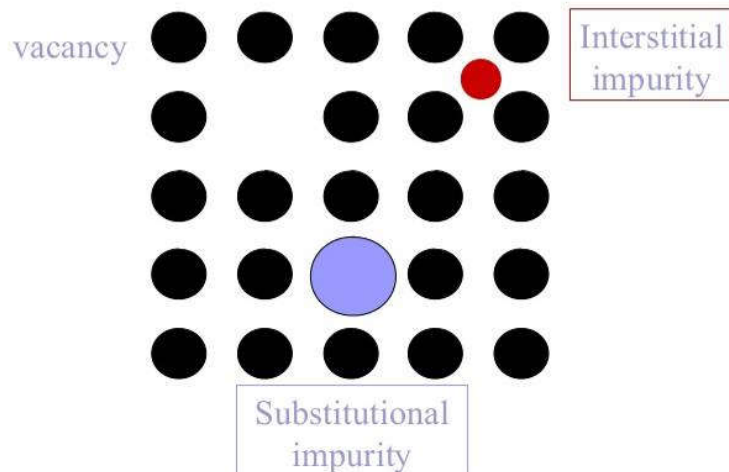
# Crystals



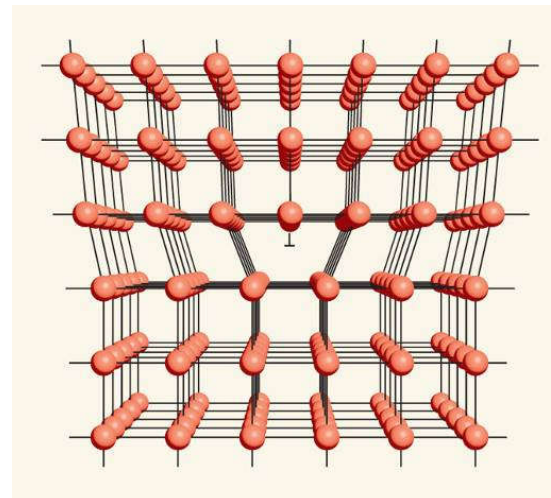
# Defects in Crystals



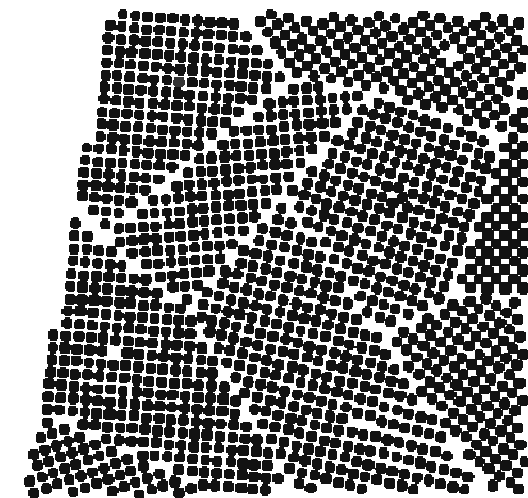
**Q: why?**



**0D**  
point defect



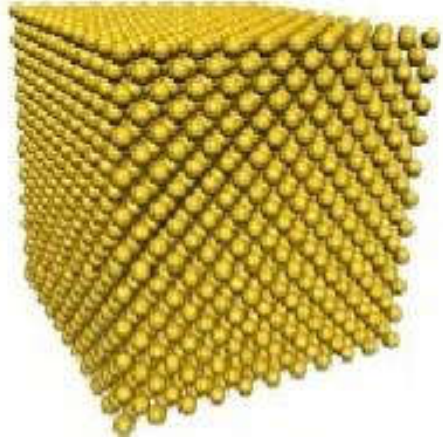
**1D**  
dislocation



**2D**  
grain boundary



# Single Crystal (Mono Crystal)



Quartz



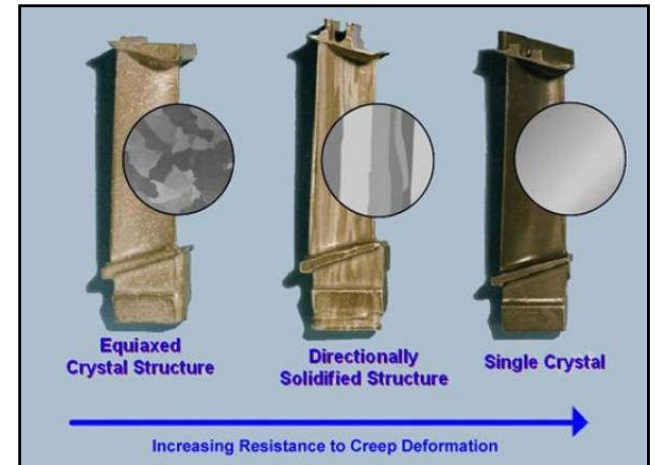
Sugar



Silicon wafers,  
GaAs, GaN, sapphire, ...

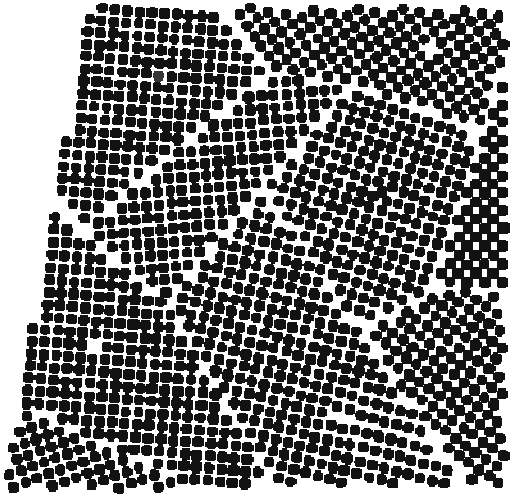


turbine blade



# Polycrystal

*Q: why blue?*

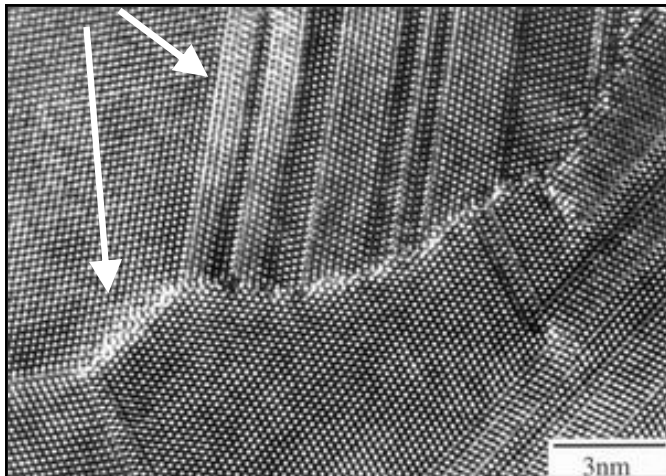


Poly-Crystalline  
Solar Cell



Mono-Crystalline  
Solar Cell

grain boundary



polycrystalline silicon



metals

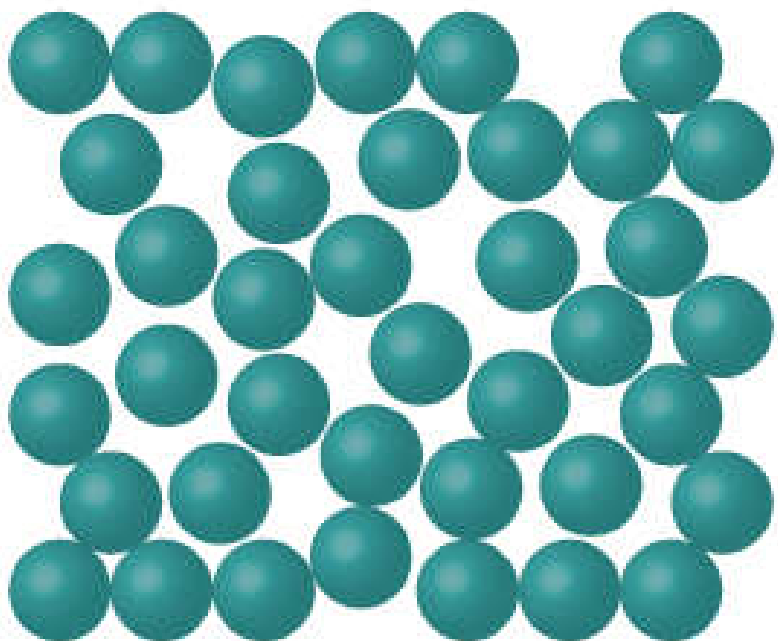


ceramics

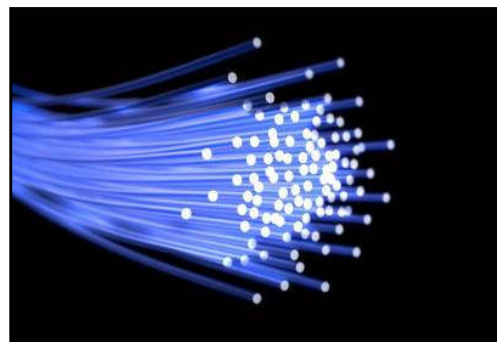


# Amorphous Materials

- Defects are everywhere ...



Amorphous



silica fiber



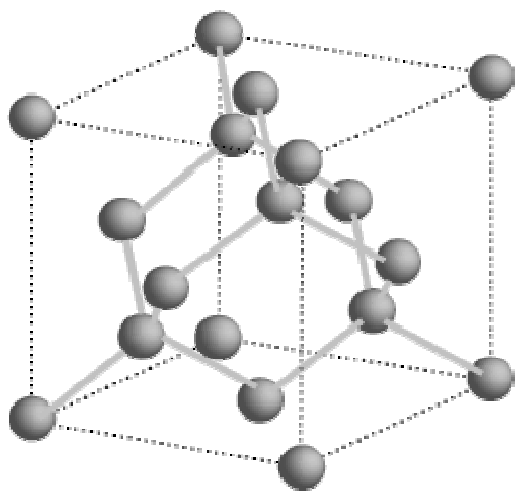
glass



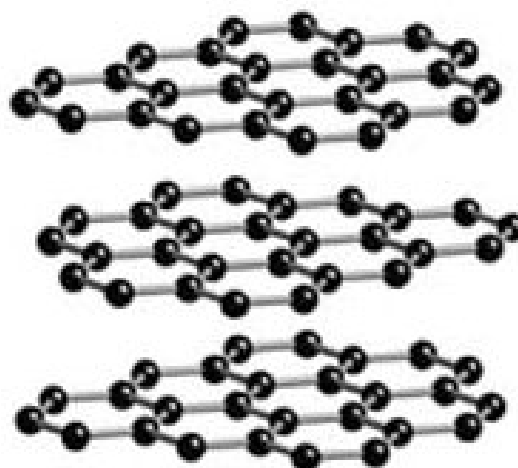
plastics

**Q: why is glass transparent?**

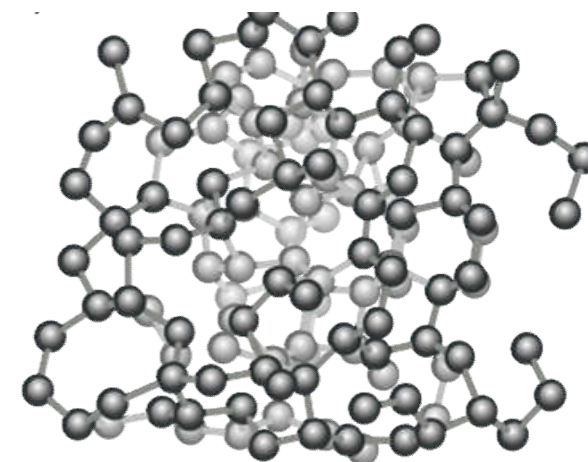
# Carbon



**diamond**



**graphite**

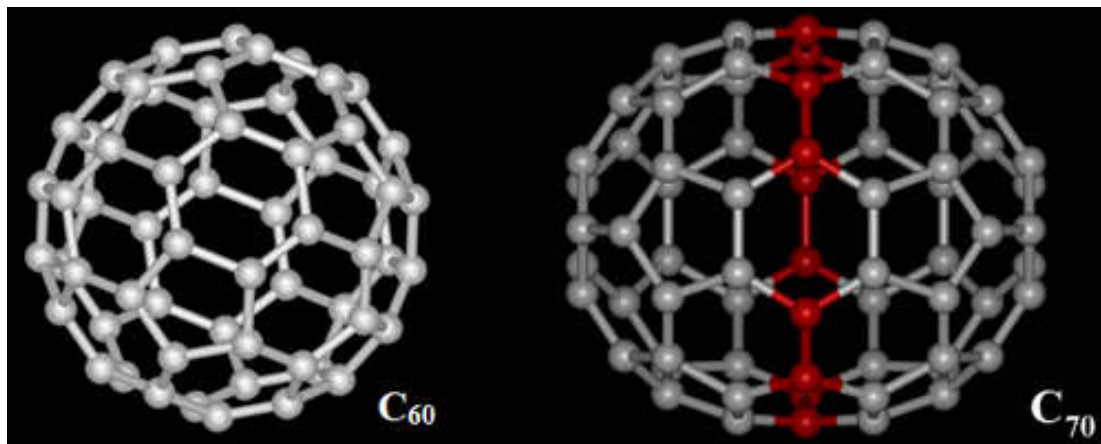


**amorphous  
carbon**

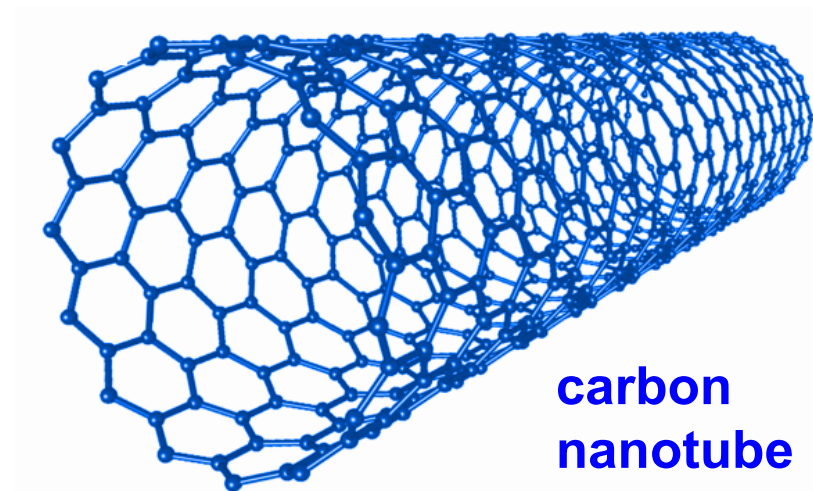
***Q: which one is electrically conductive, diamond or graphite?***



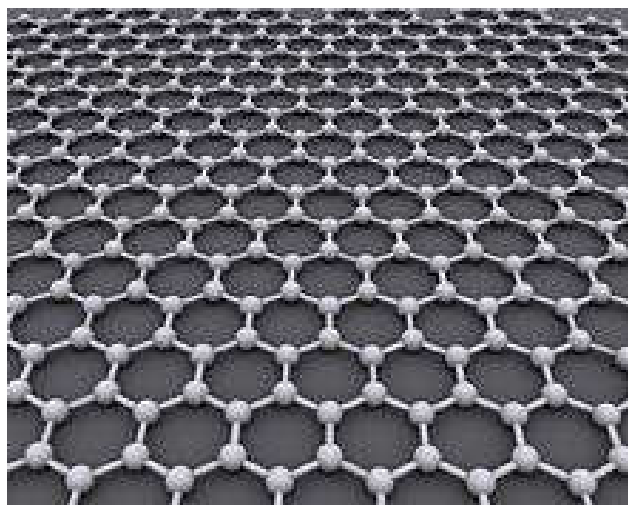
# Carbon



**H. Kroto, R. Curl, R. Smalley**  
**1996 Nobel Prize in Chemistry**



S. Iijima, *Nature* **354**, 56 (1991)

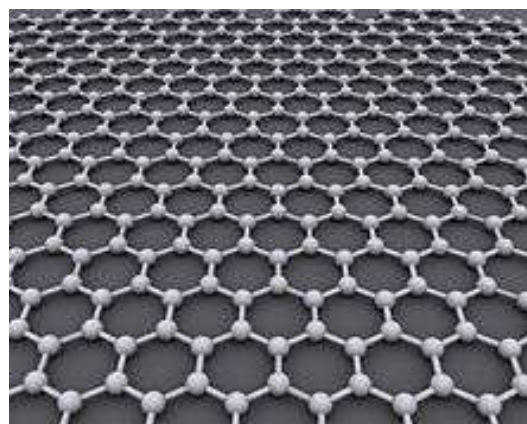


**graphene**

**A. Geim, K. Novoselov**  
**2010 Nobel Prize in Physics**

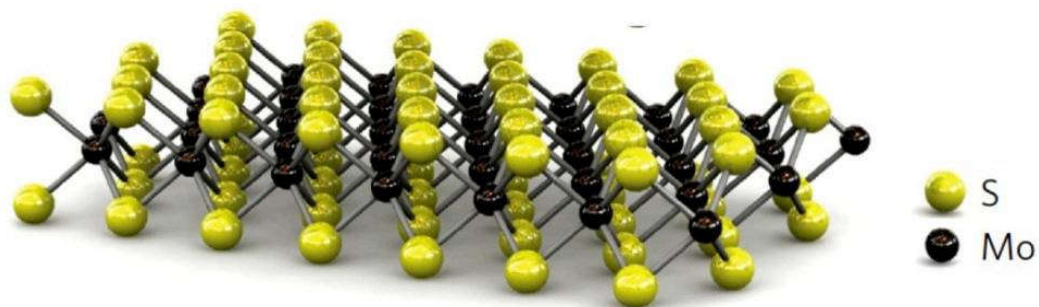
# 2D Materials

- Single atomic layer crystal

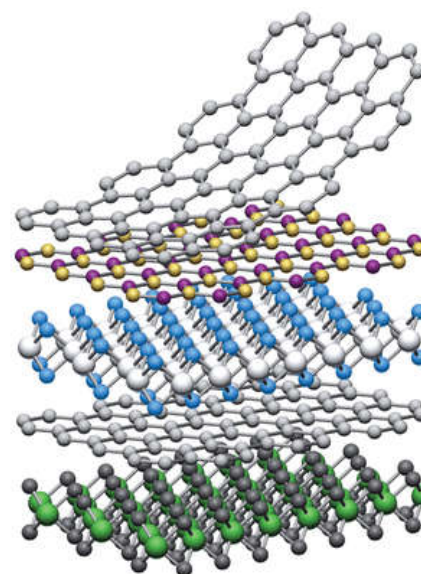


graphene

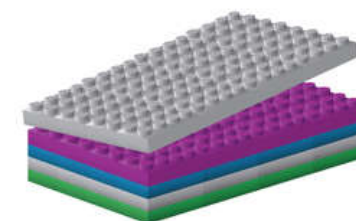
**A. Geim, K. Novoselov**  
**2010 Nobel Prize in Physics**



**Transition metal dichalcogenide (TMDC)**  
**MoS<sub>2</sub>, WSe<sub>2</sub>, ...**

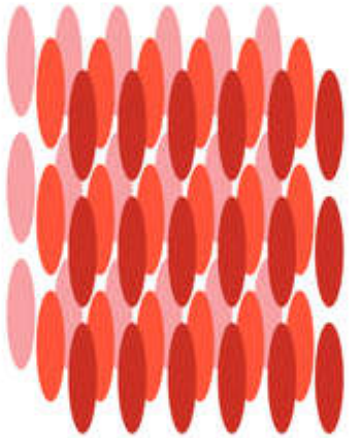


	Graphene	
	hBN	
	MoS <sub>2</sub>	
	WSe <sub>2</sub>	
	Fluorographene	



# Liquid Crystals

Crystalline Solid



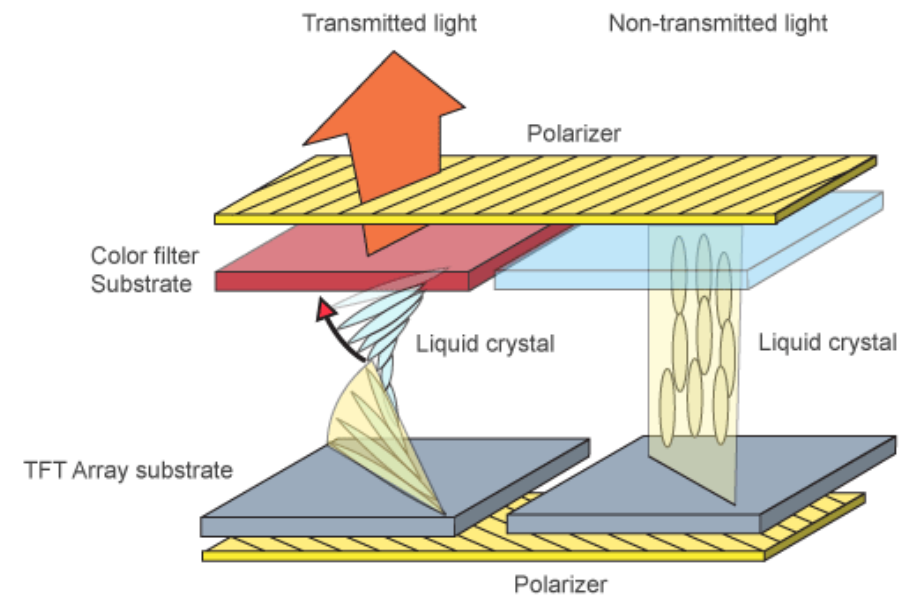
Liquid Crystal



Isotropic Liquid



## Liquid crystal display (LCD)



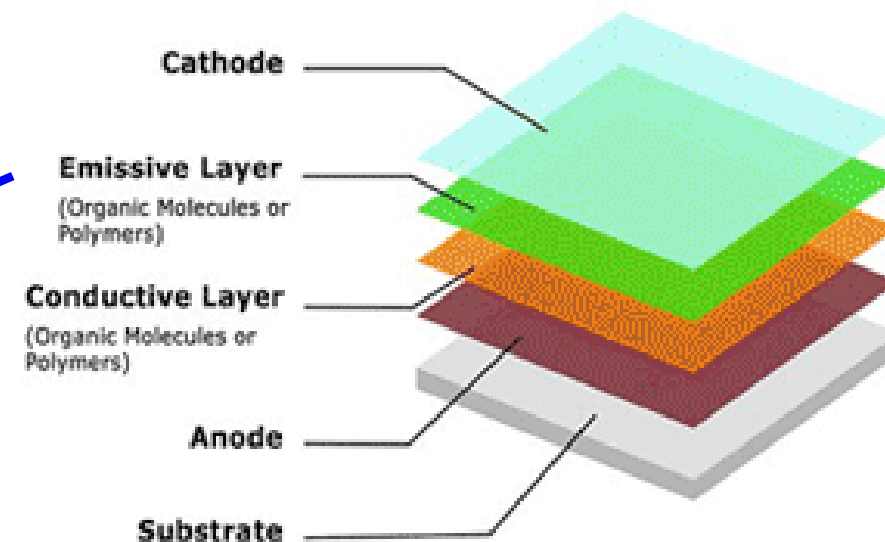
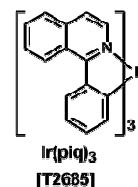
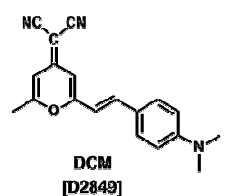
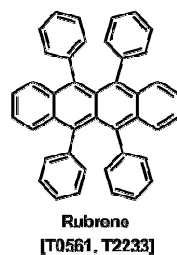
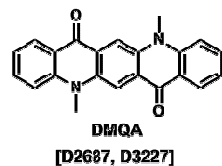
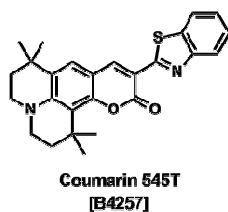
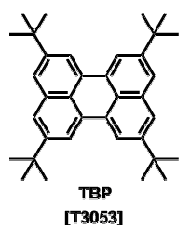
**P. de Gennes**  
**1991 Nobel Prize in Physics**

Diagram 2: The Fundamental Photonics of Liquid Crystal (Twisted Nematics)

# Organic Materials

## Small Molecules

### OLED Dopants



# OLED

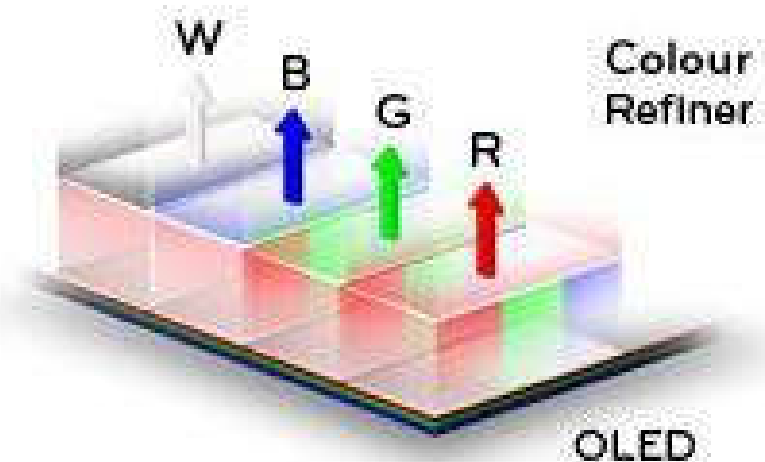
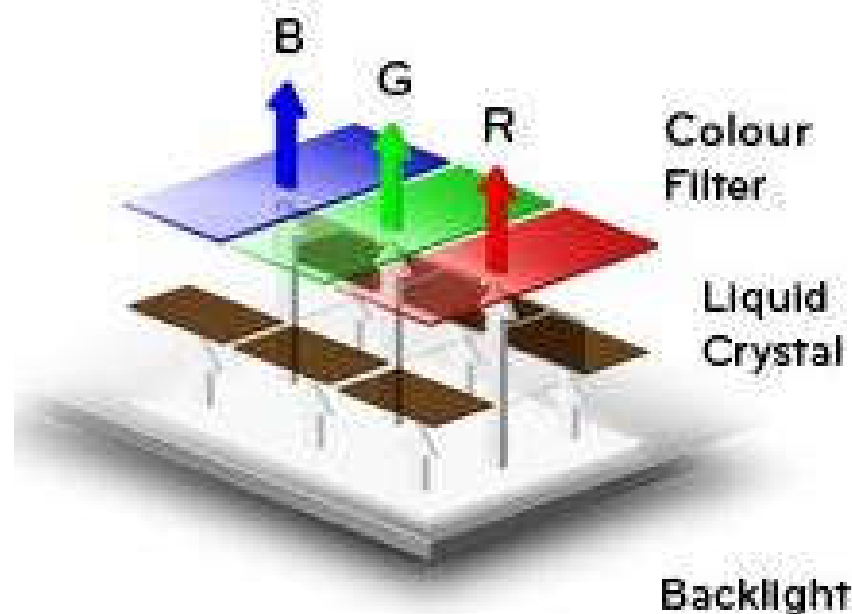


# Organic Materials

## LCD

## vs.

## OLED

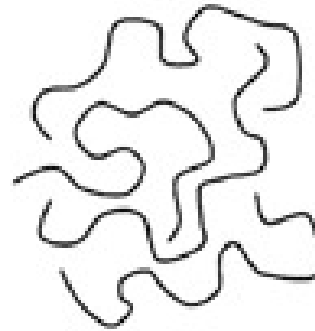
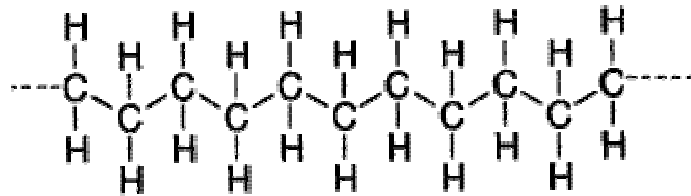


- Complex Structure
- BLU (Backlight Unit) CCFL, LED
- Lighting Unit = Pixel Unit

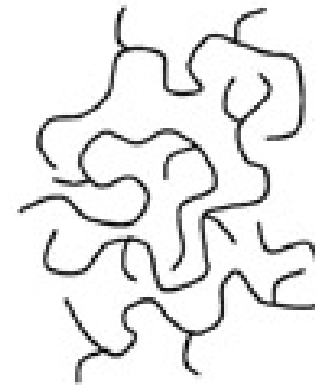
- Simple Structure
- Self-emissive
- Lighting Unit = Pixel Unit

# Organic Materials

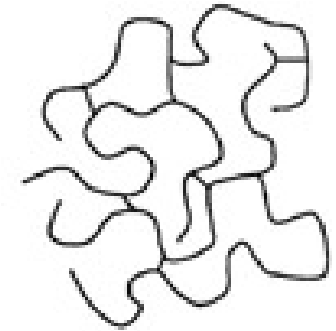
## ■ Polymers



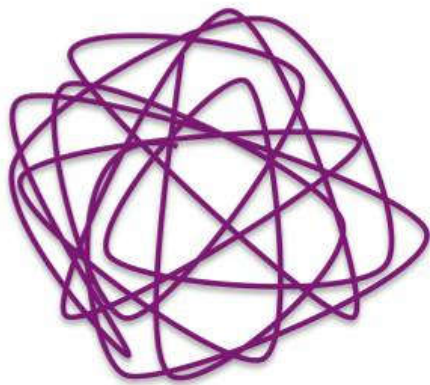
Linear



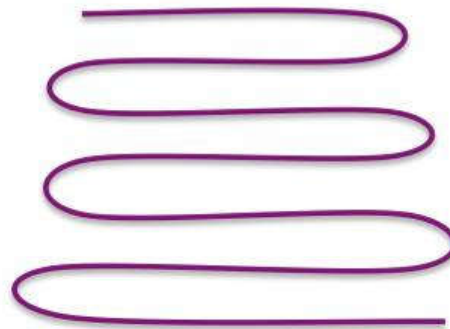
Branched



Cross-linked

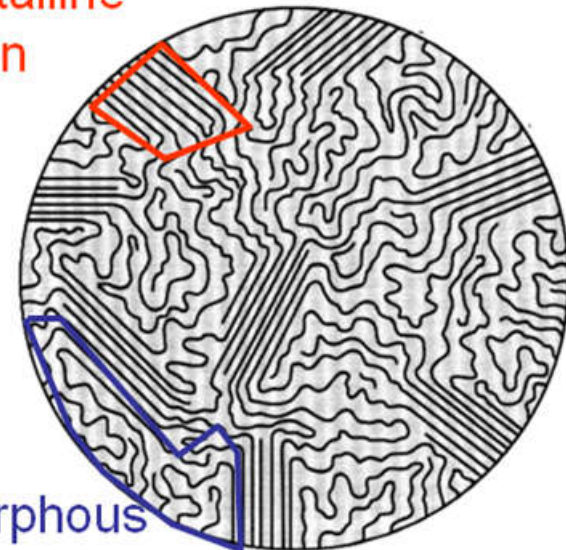


Amorphous



Crystalline

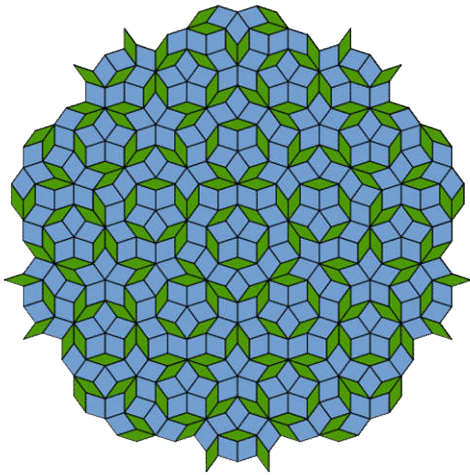
Crystalline  
region



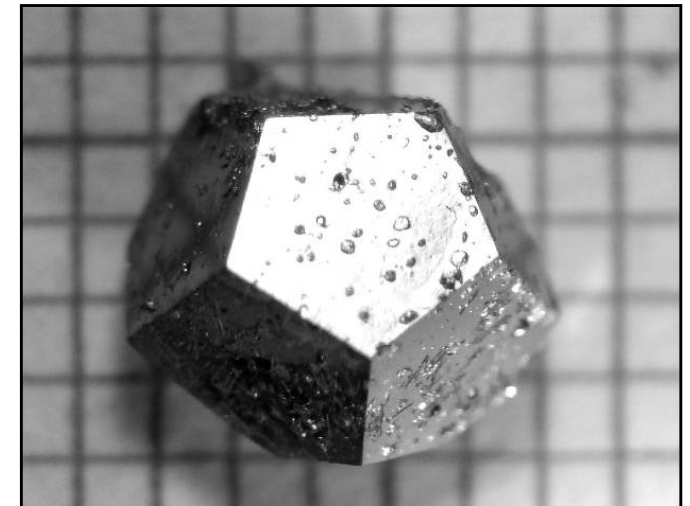
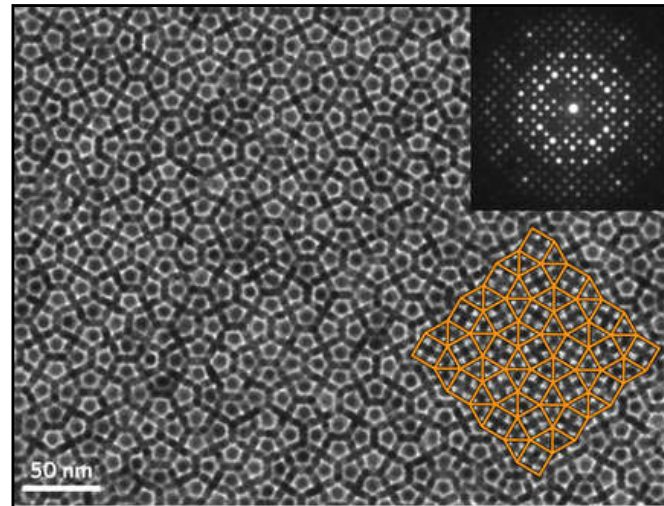
Amorphous  
region

# Quasi-Crystal

- **Neither crystalline nor amorphous**
  - **5, 8, 10, or 12-fold symmetry**



Penrose tiling



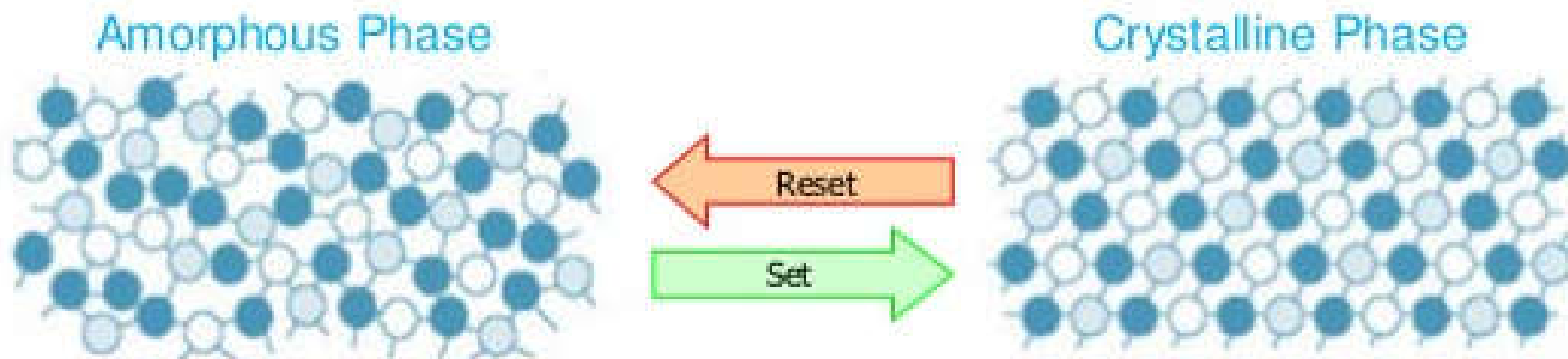
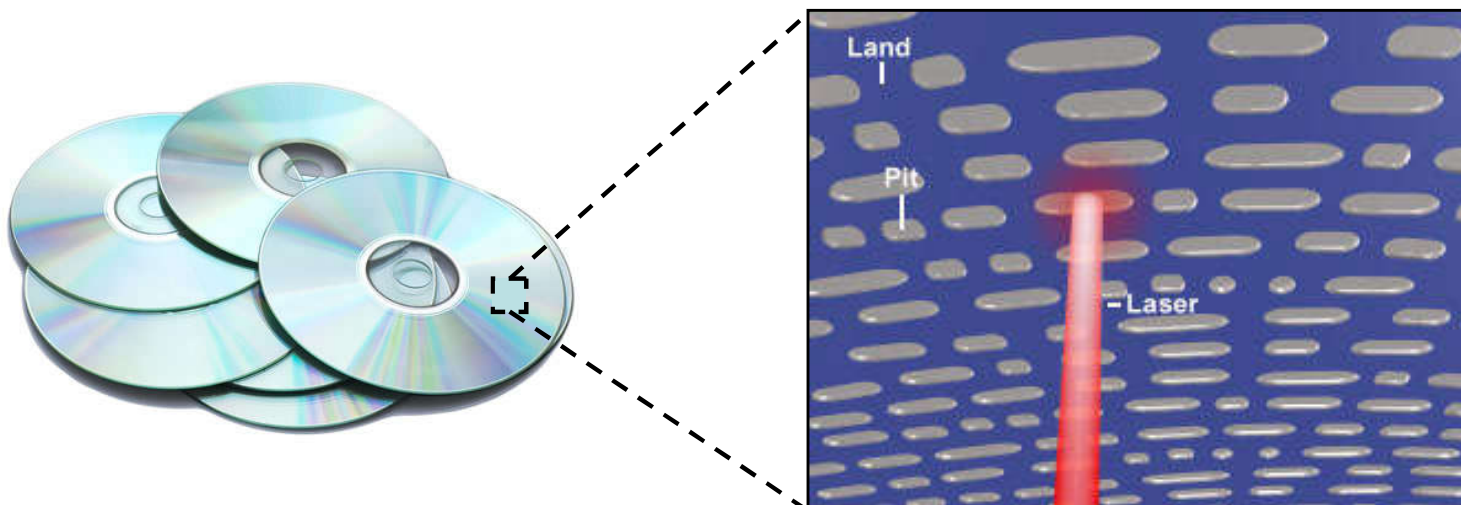
A Ho-Mg-Zn quasicrystal



**D. Shechtman**  
**2011 Nobel Prize in Chemistry**

# Optical Disc

- Phase Change Memory





# Materials Characterization

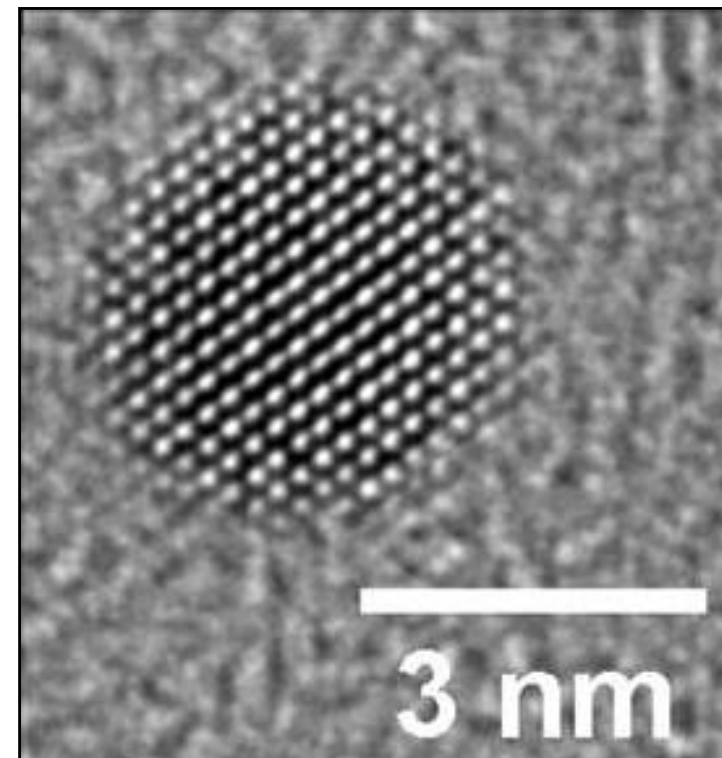
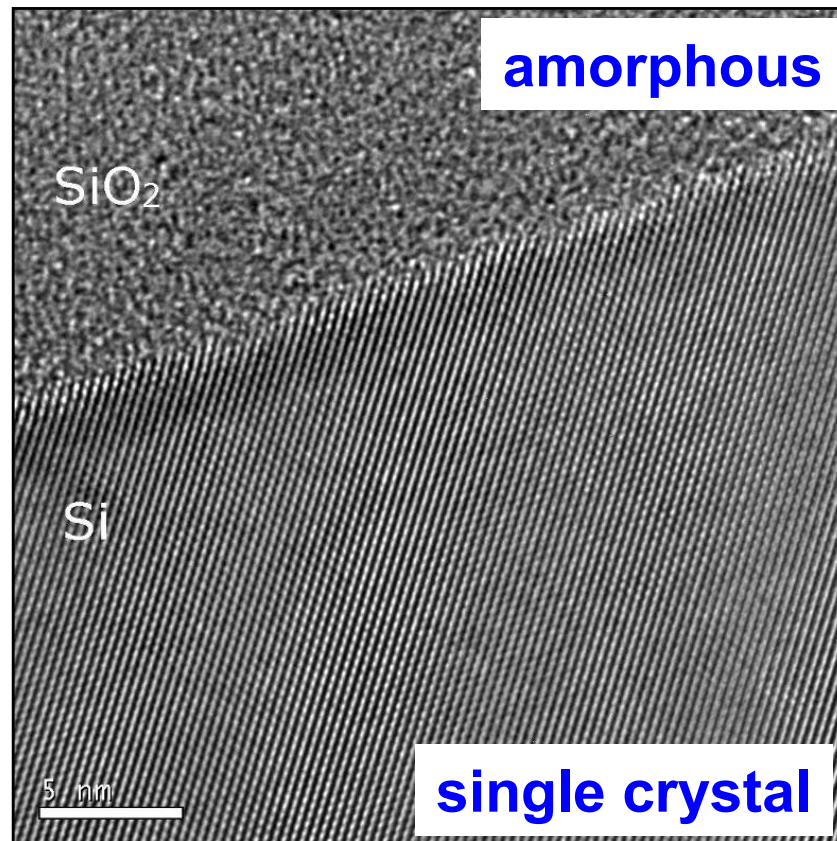
---

- **SEM / TEM**
  - **Scanning / Transmission Electron Microscope**
  
- **HRTEM**
  - **High Resolution Transmission Electron Microscope**
  
- **XRD**
  - **X-ray Diffraction**
  
- **DSC**
  - **Differential Scanning Calorimetry**

# Materials Characterization

## ■ HRTEM

- High Resolution Transmission Electron Microscope

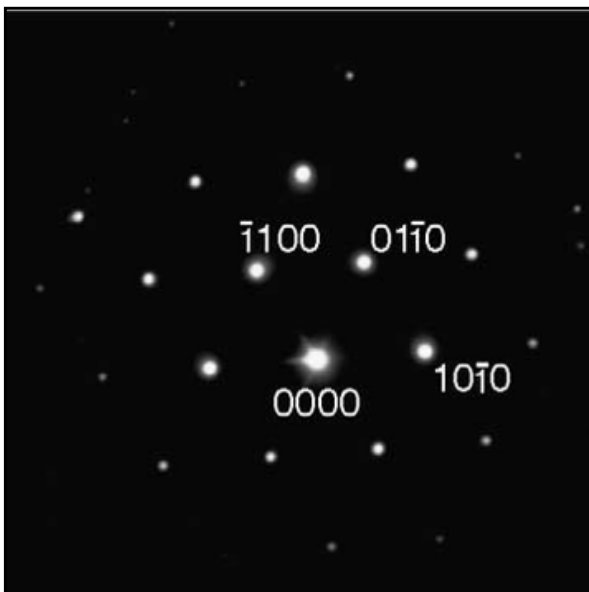


quantum dot

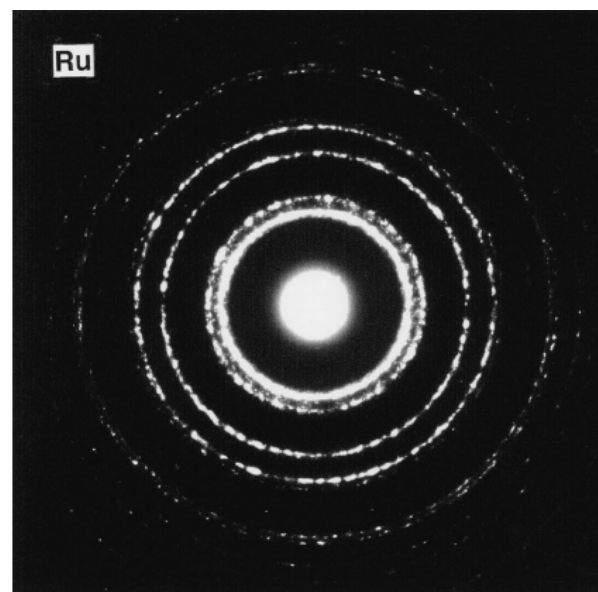
# Materials Characterization

- HRTEM
  - High Resolution Transmission Electron Microscope

## diffraction patterns



single crystal



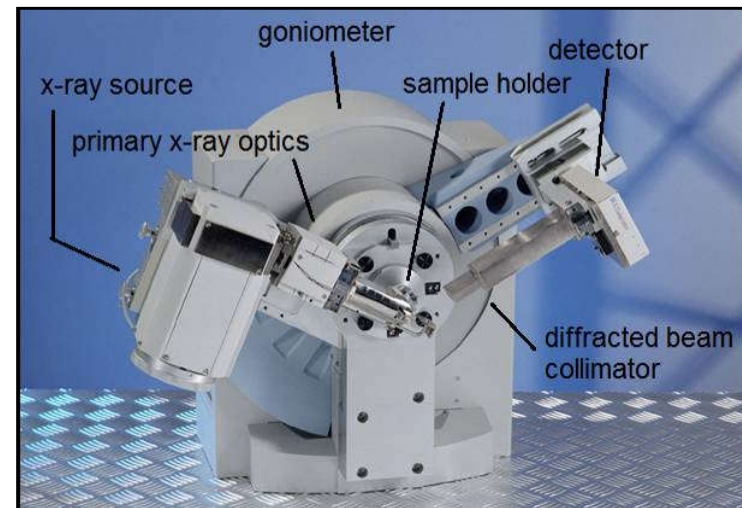
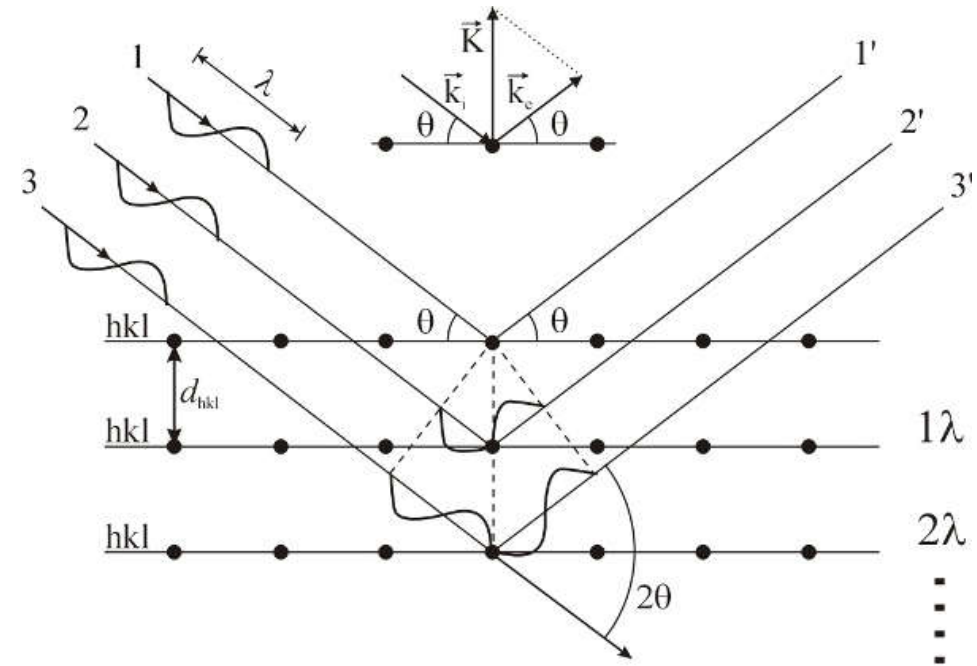
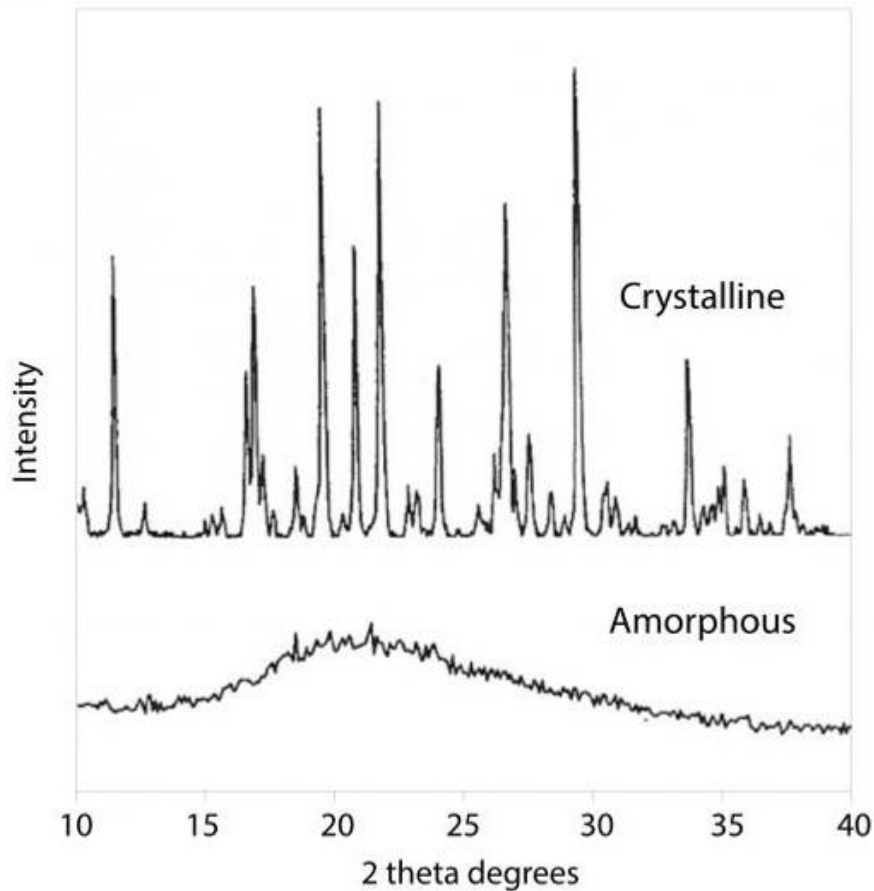
polycrystal



amorphous

# Materials Characterization

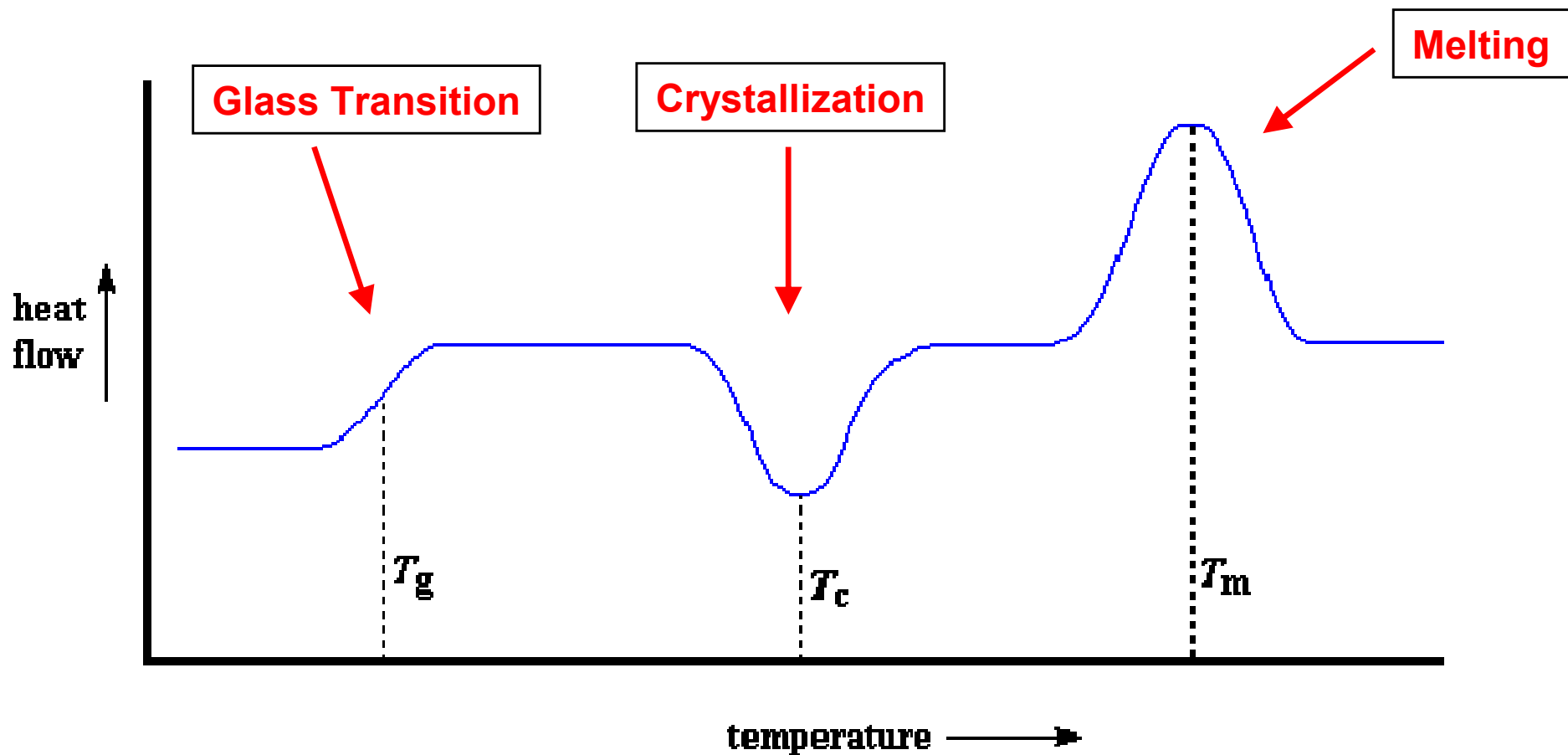
- XRD
  - X-ray Diffraction



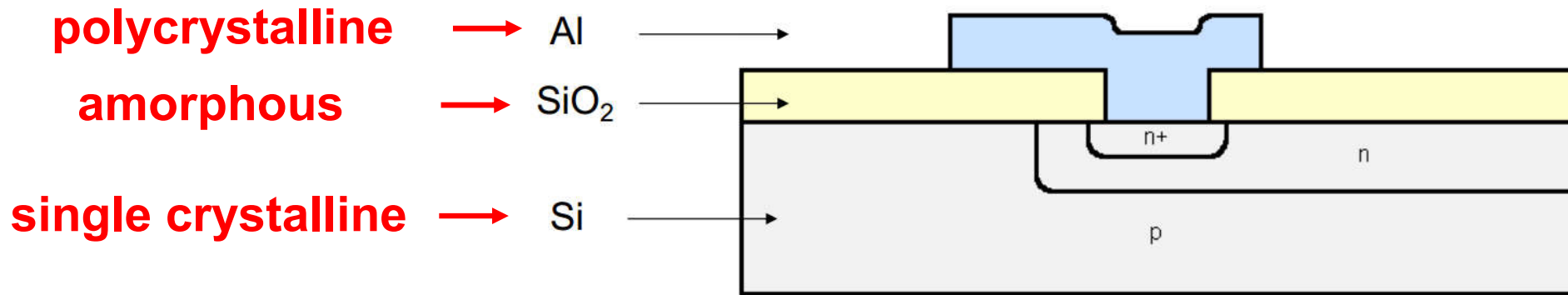


# Materials Characterization

- DSC
  - Differential Scanning Calorimetry



# CMOS Device



**Silicon**



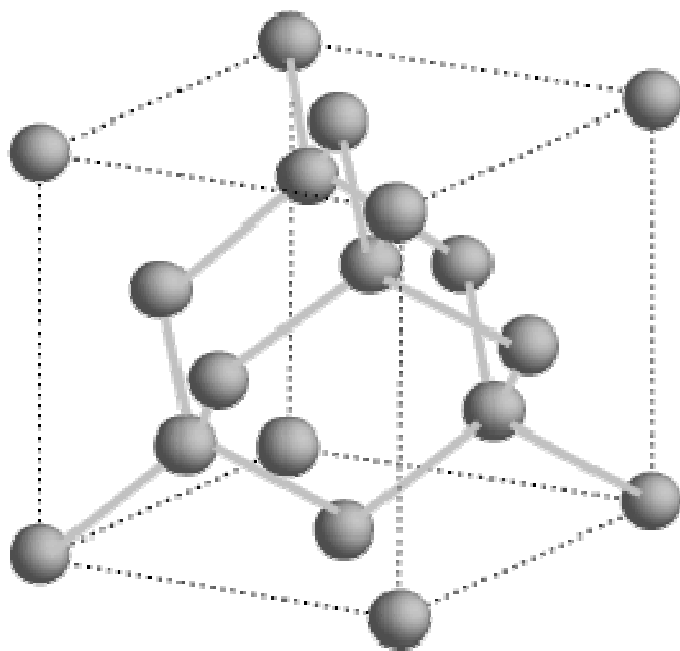
**SiO<sub>2</sub>**



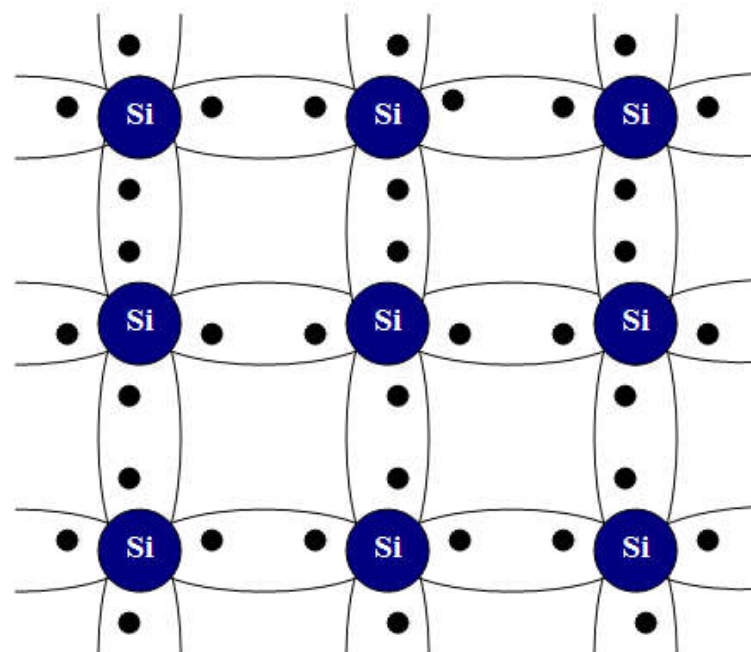
**Metal**

# Substrates for Devices

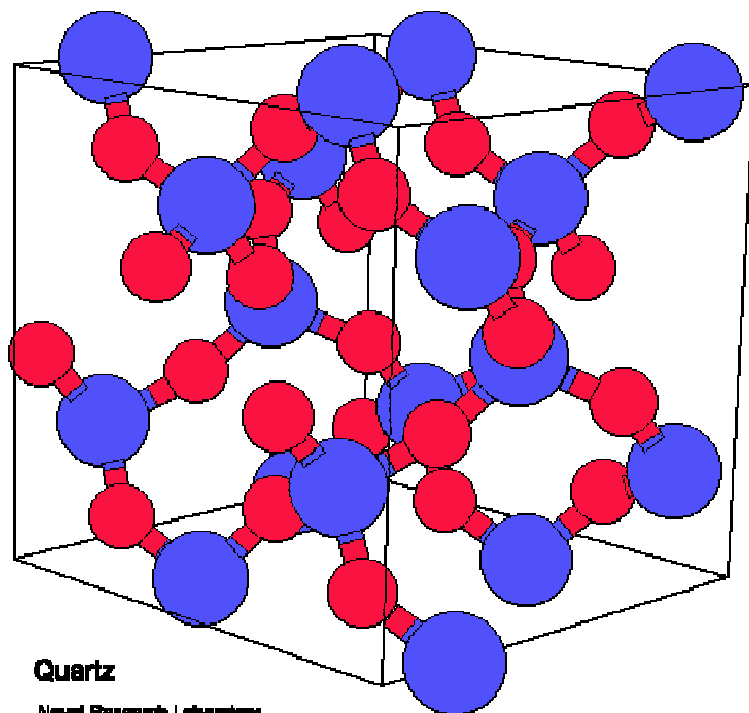
- Usually single crystals



diamond structure:  
Si, Ge, C, ...



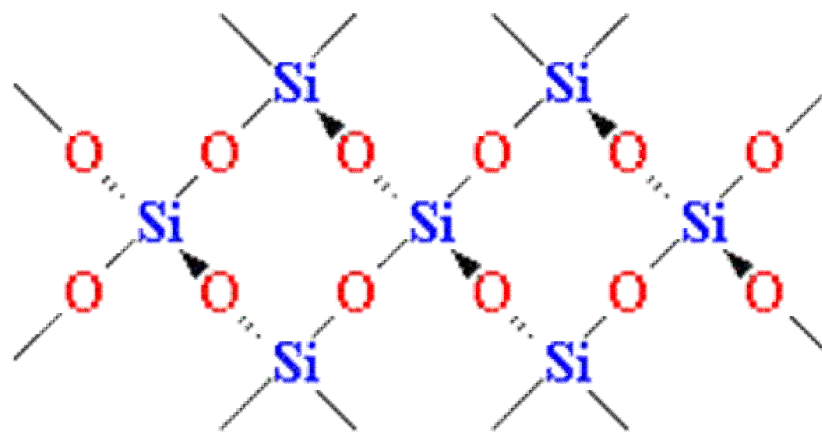
# Substrates for Devices



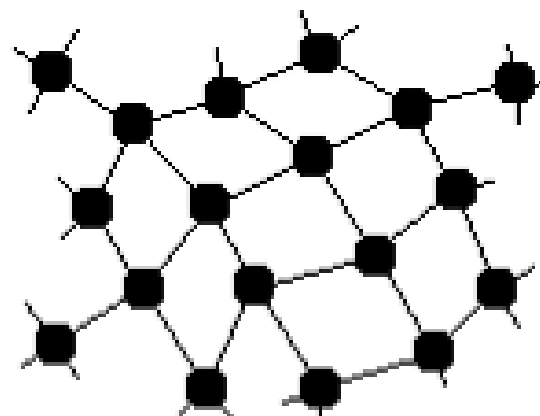
Quartz

Naval Research Laboratory  
Center for Computational Materials Science

quartz (SiO<sub>2</sub>)  
single crystalline

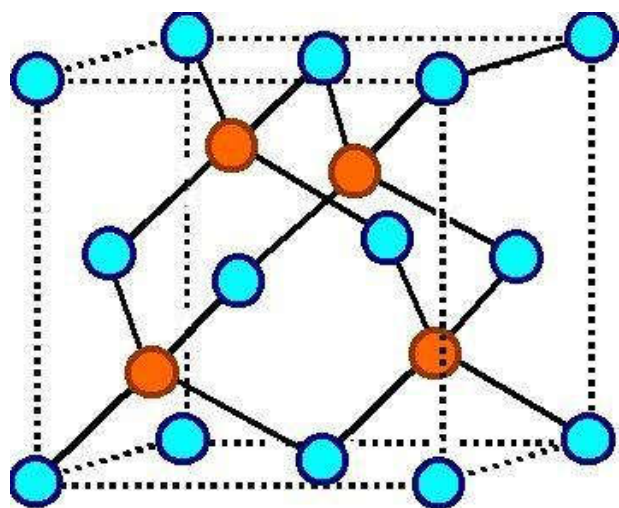


amorphous  
glass

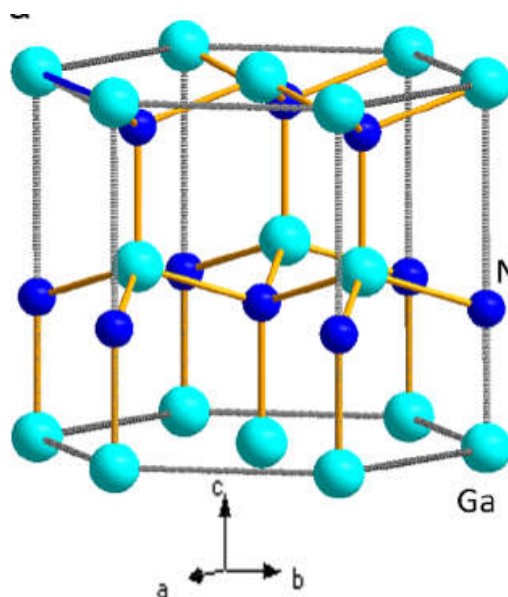




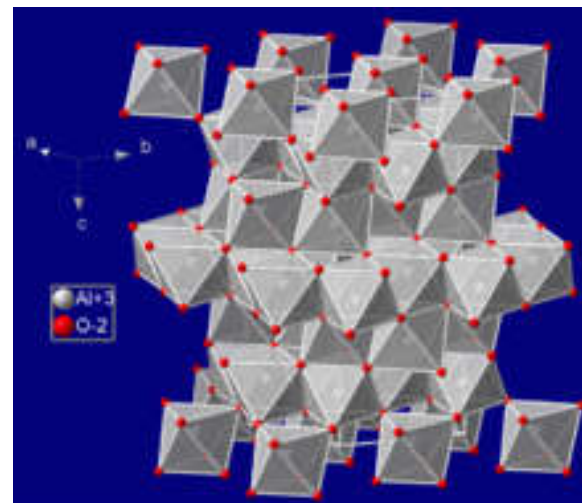
# Substrates for Devices



zinc blende structure:  
GaAs, InP,  $\beta$ -SiC, ...

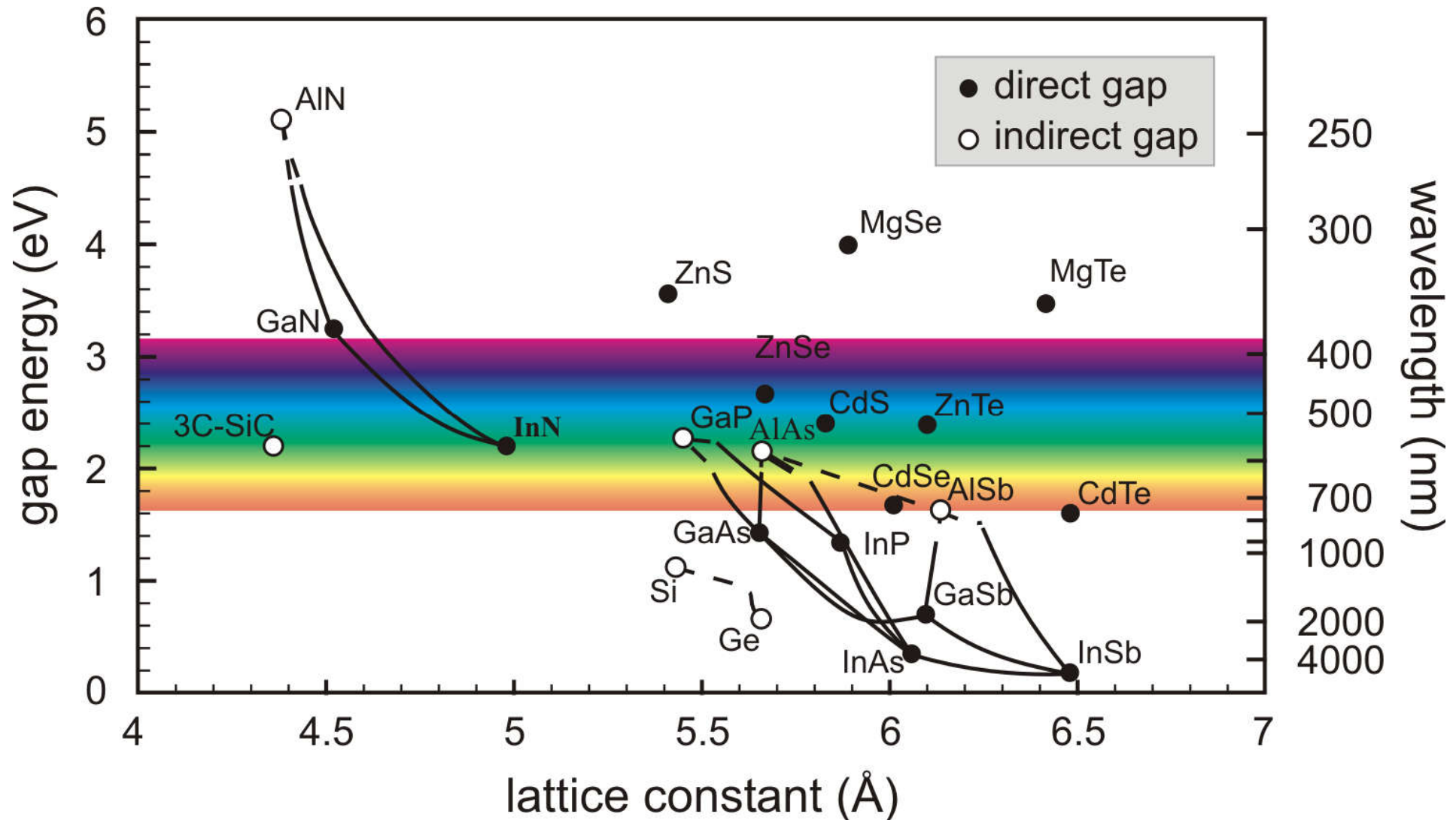


Wurtzite structure:  
 $\alpha$ -SiC, GaN, ZnO, ...



sapphire ( $\text{Al}_2\text{O}_3$ )

# Lattice Constants vs. Bandgap



# Requirement for Electronics

---

- **low cost**
- **single crystal**
- **p-doping and n-doping**
- **low defect level**
  - **purity > 99.99999....%**
  - **dislocation < 1000 /cm<sup>2</sup>**
- **suitable bandgap**
  - **too large -> high voltage, power, ...**
  - **too small -> thermal noise, leakage, defects, ...**
- **semiconductor/oxide interface quality**
- **mobility, surface uniformity, ...**

# Silicon vs. Germanium

## Silicon

- earth abundant
  - > 25% on earth
- perfect Si/SiO<sub>2</sub> interface
- bandgap 1.1 eV

VS.

## Germanium

- expensive
- GeO<sub>2</sub> is not stable
- bandgap 0.67 eV

***Silicon wins  
and will always win (?)***



# Properties of Silicon

## ■ Structural

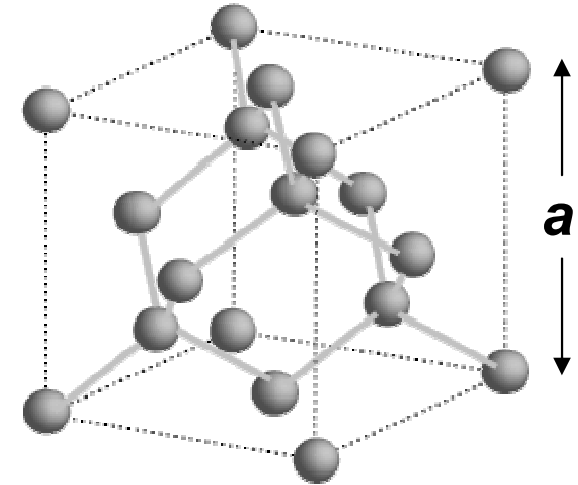
- ❑ diamond structure (FCC)
- ❑ lattice constant  $a = 5.431 \text{ \AA}$
- ❑ atomic density =  $5 * 10^{22} / \text{cm}^3$
- ❑ melting point =  $1417 \text{ }^\circ\text{C}$

## ■ Electronic

- ❑ bandgap  $E_g = 1.12 \text{ eV}$
- ❑ dielectric constant  $\epsilon_r = 11.9$
- ❑ mobility: electron  $\mu_e = 1500 \text{ cm}^2/\text{V/s}$ , hole  $\mu_h = 450 \text{ cm}^2/\text{V/s}$
- ❑ intrinsic carrier density  $n_i = 1.45 * 10^{10} / \text{cm}^3$

## ■ Optical

- ❑ refractive index  $n = 3.6$
- ❑ absorbs  $< 1100 \text{ nm}$ , transparent  $> 1100 \text{ nm}$



# How to Make Silicon Wafers?

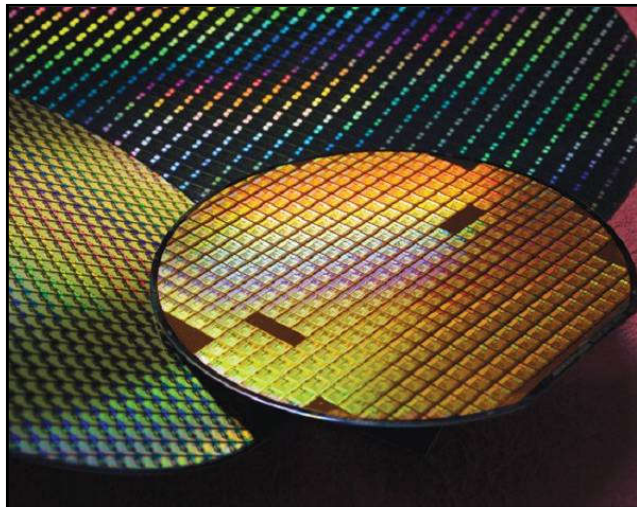


$\text{SiO}_2$



raw Si

[Video](#)



IC chips



Si ingots and wafers

# How to Make Silicon Wafers?



$\text{SiO}_2$



raw Si



**Metallurgical Grade Silicon, purity ~ 98%**  
**Applications: aluminum, silicone, ...**

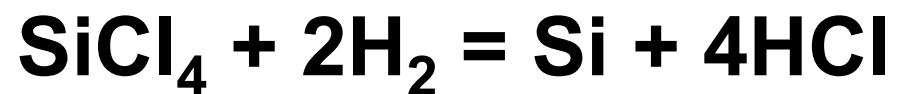
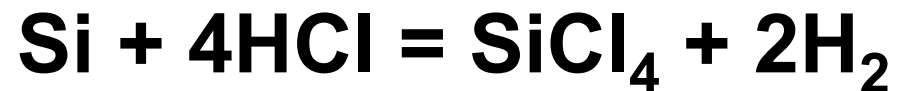
# How to Make Silicon Wafers?



$\text{SiO}_2$



raw Si



**purification  
(Siemens process)**



**Polycrystalline Silicon, purity > 99.99%**

**Applications: solar cells, ...**



# How to Make Silicon Wafers?

poly crystal -> single crystal

Czochralski process (CZ)

Float-zone process (FZ)



raw Si

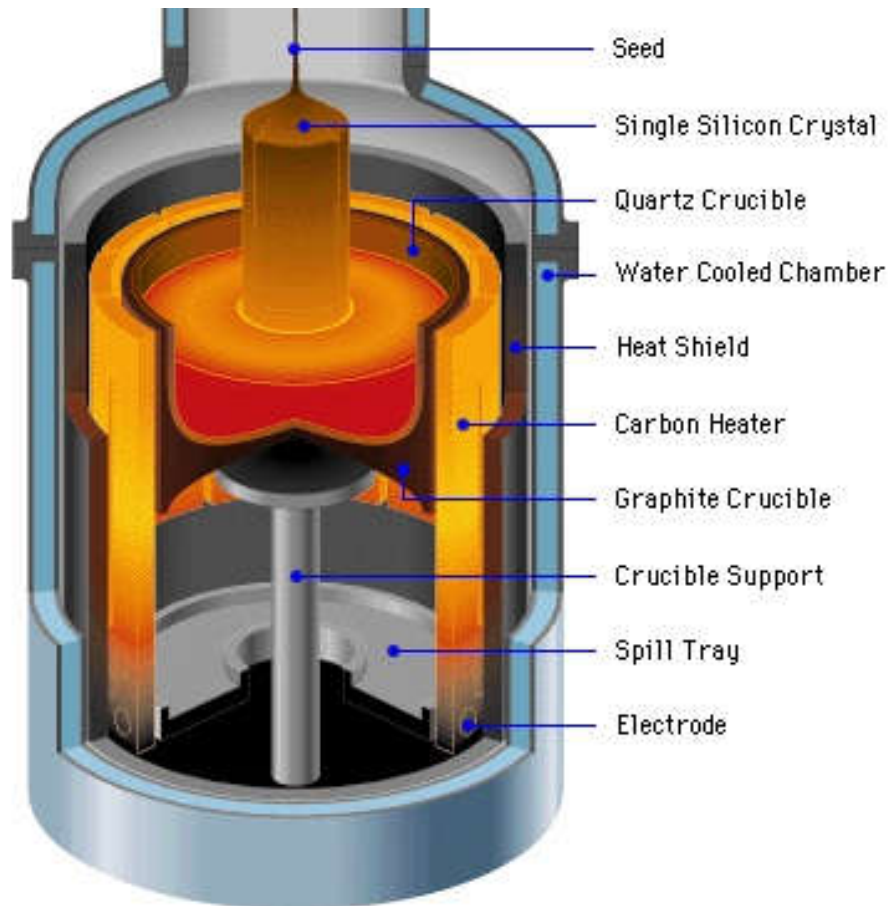


Si ingots and wafers

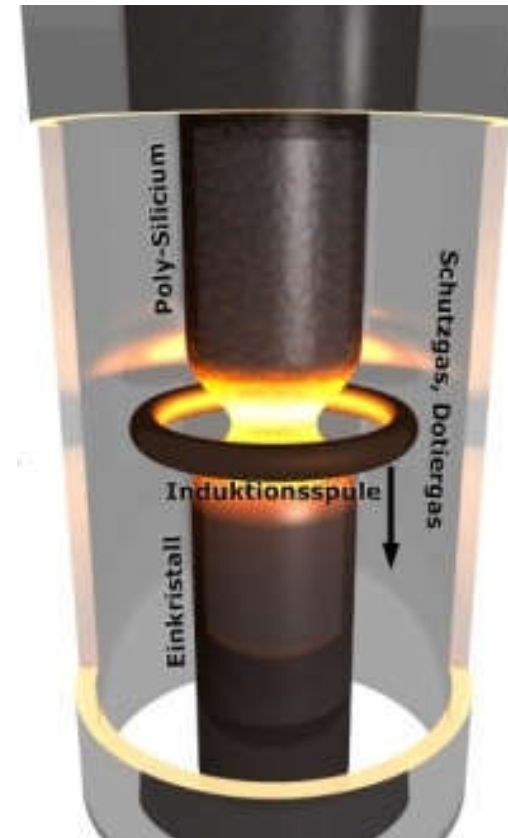


# How to Make Silicon Wafers?

## Czochralski process (CZ)

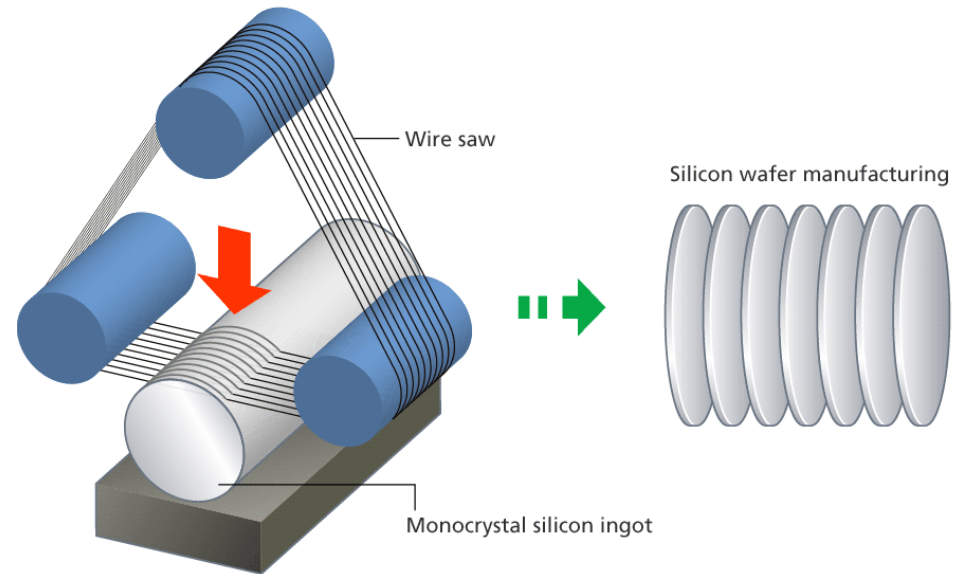


## Float-zone process (FZ)

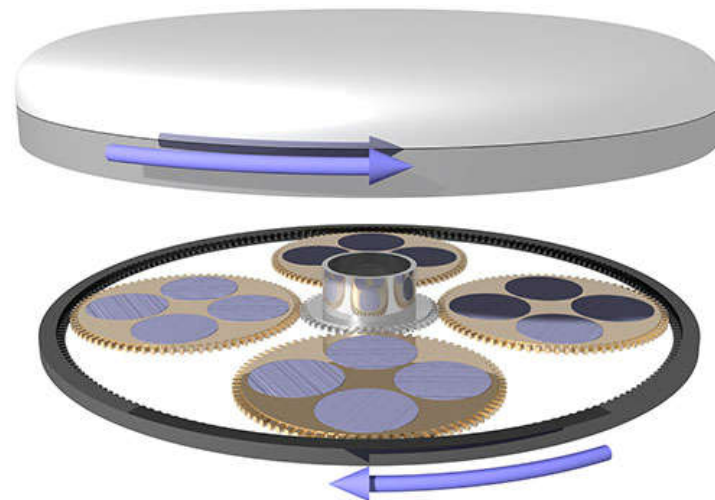


# How to Make Silicon Wafers?

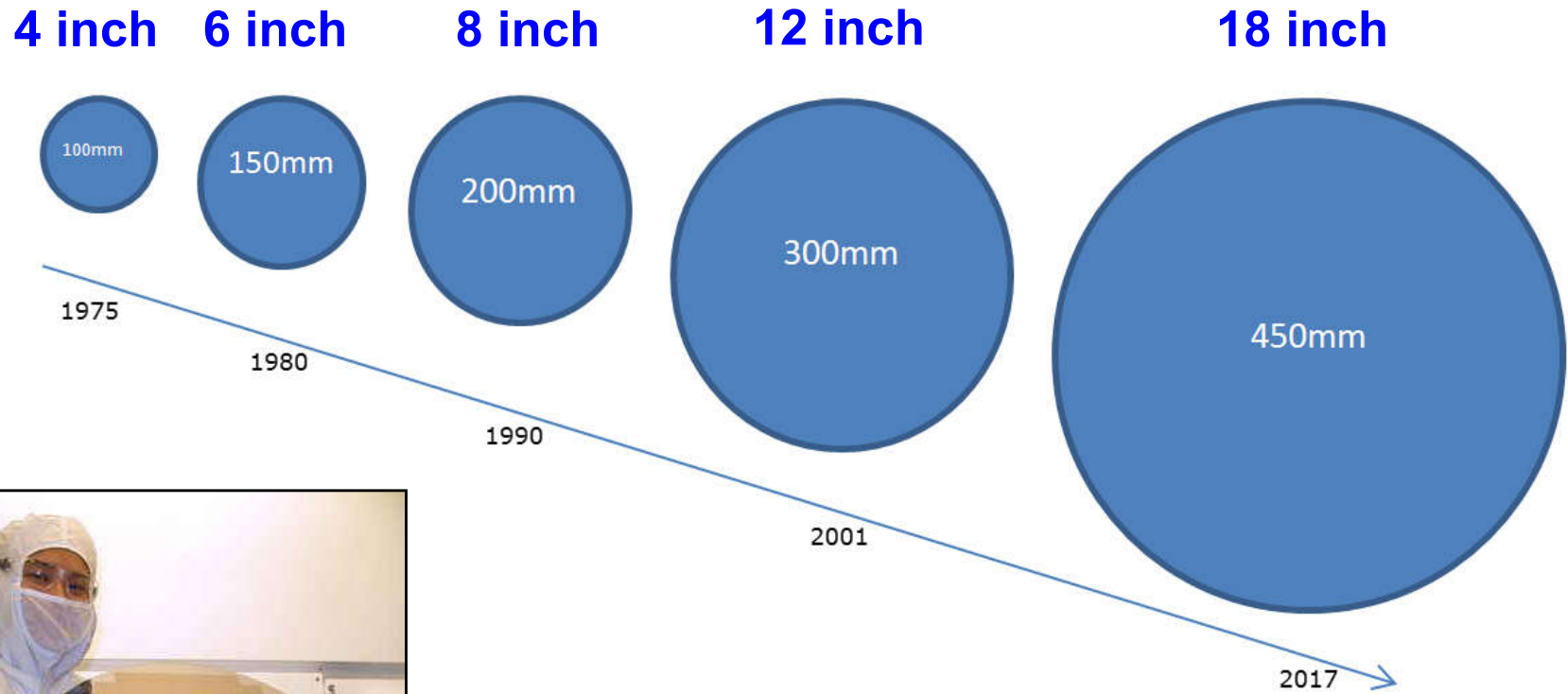
**wafer slicing**



**wafer polishing**



# Silicon wafers: size



**18 inch wafer**

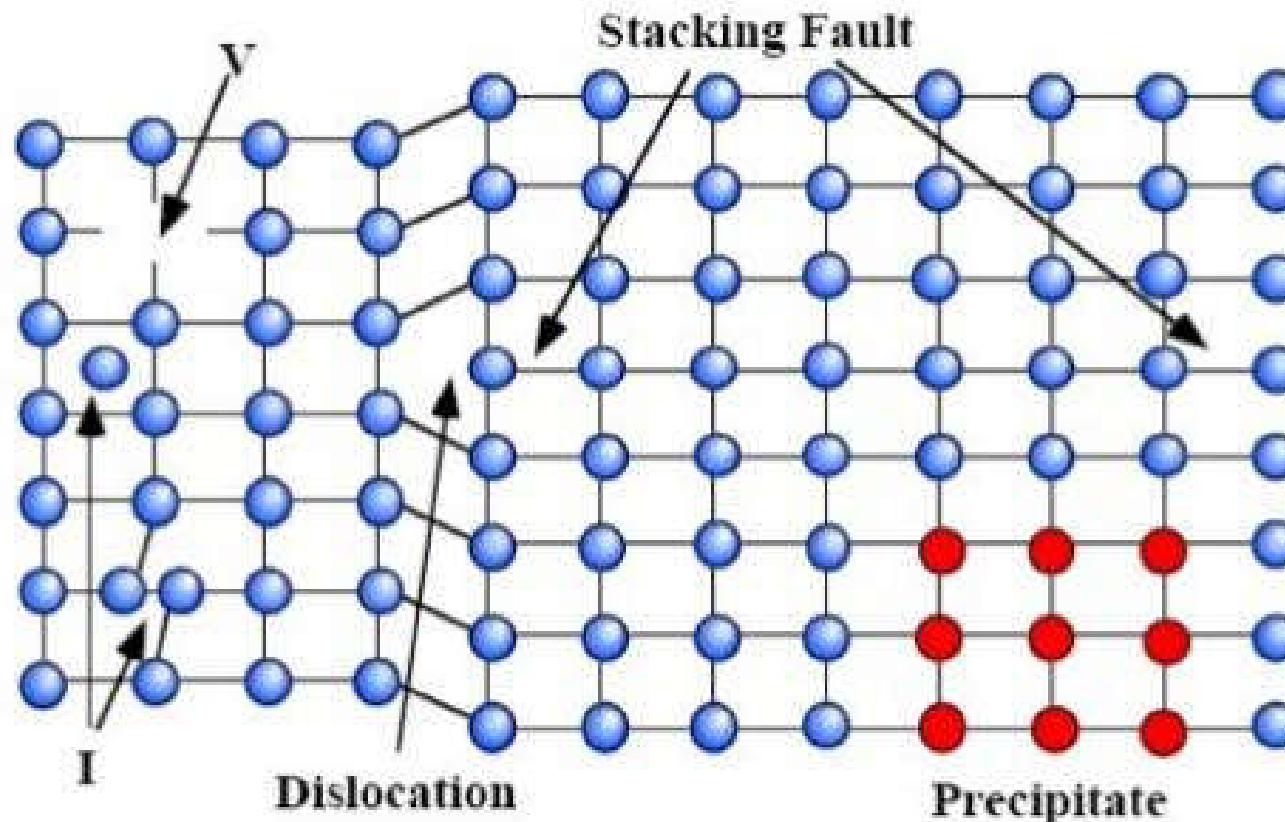
# Silicon wafers: purity

---

- **Metallurgical grade**
  - polycrystalline
  - purity > 98%
  - application: aluminum alloy, silicone
  
- **Solar grade**
  - polycrystalline
  - purity > 99.99% (4N)
  - application: solar cells
  
- **Electronic grade**
  - single crystalline
  - purity > 99.9999999% (9N)
  - application: IC industry, high efficiency solar cells

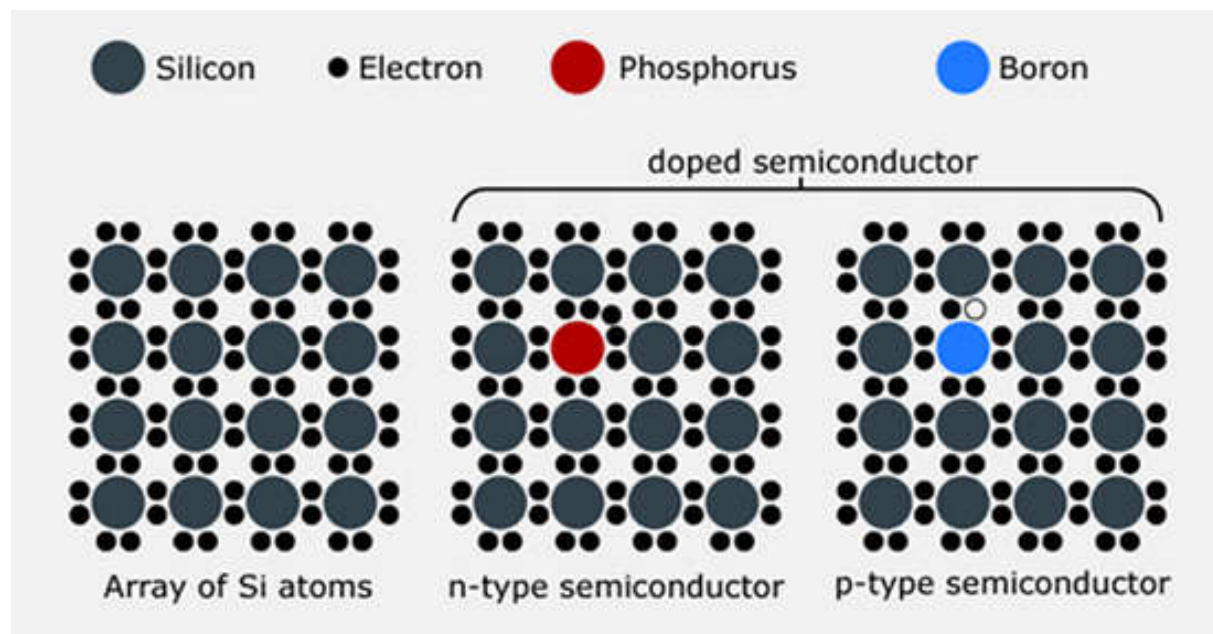
# Silicon wafers: defects

- Point Defects e.g. Vacancies (V), Interstitials (I)
- Line Defects e.g. Dislocations
- Area Defects e.g. Stacking Faults (“extrinsic” or “intrinsic” form along {111} planes)
- Volume Defects e.g. Precipitates, Collection of Vacancies

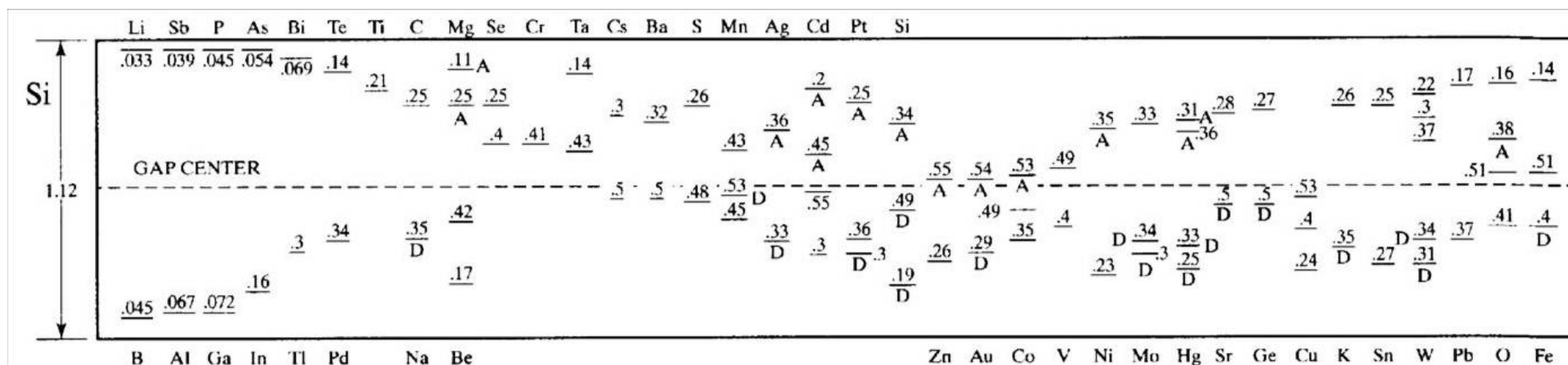




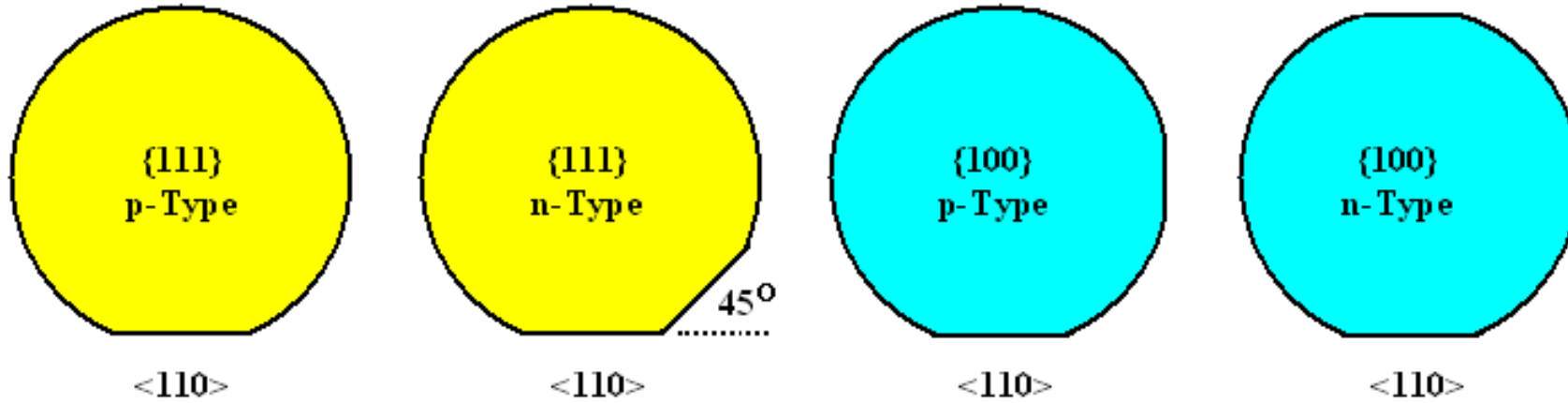
# Silicon wafers: doping



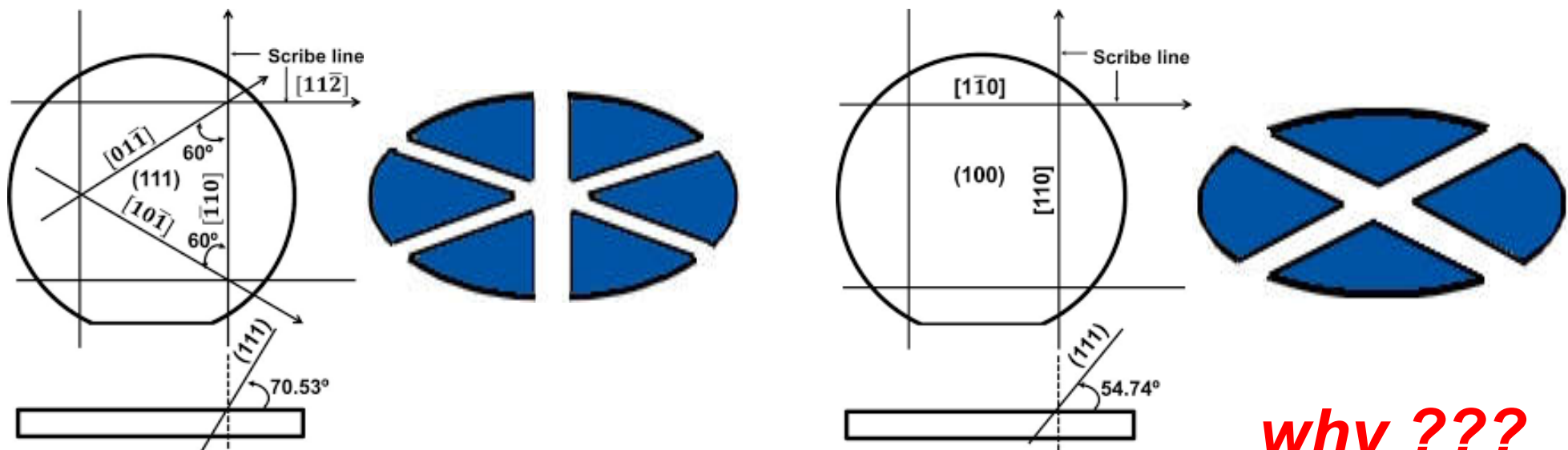
					2
	5	6	7	8	9
	B	C	N	O	F
	13	14	15	16	17
	Al	Si	P	S	Cl
	31	32	33	34	35
	Ga	Ge	As	Se	Br
	49	50	51	52	53
	In	Sn	Sb	Te	I
	81	82	83	84	85
	Tl	Pb	Bi	Po	At
					86
					Rn



# Silicon wafers: orientation

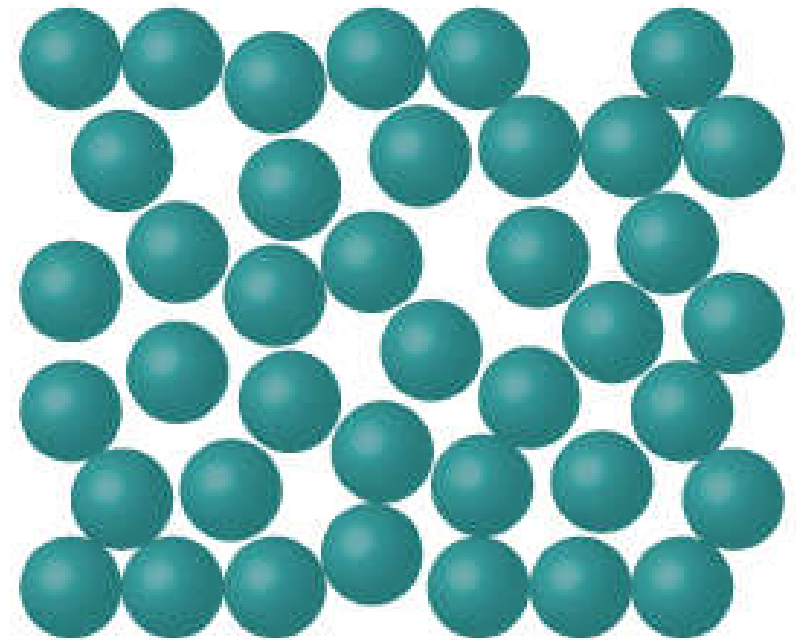
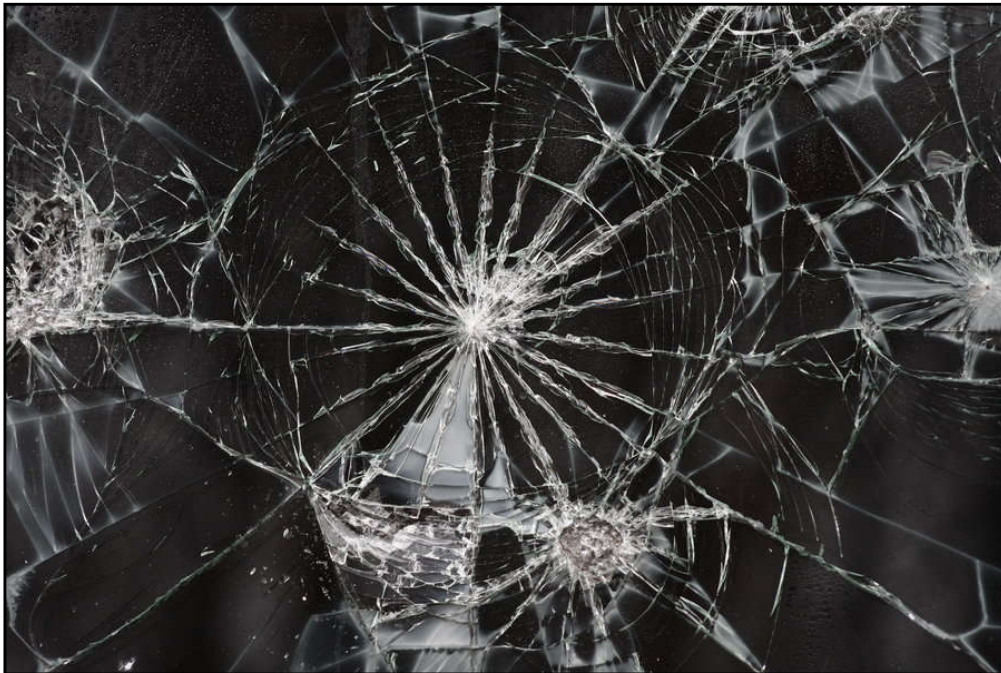


## cleavage direction



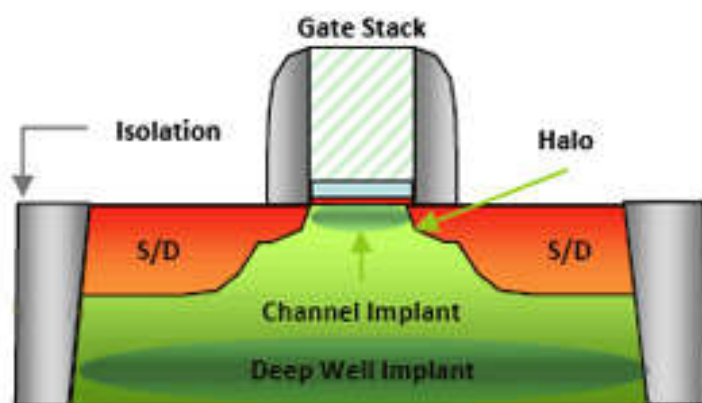
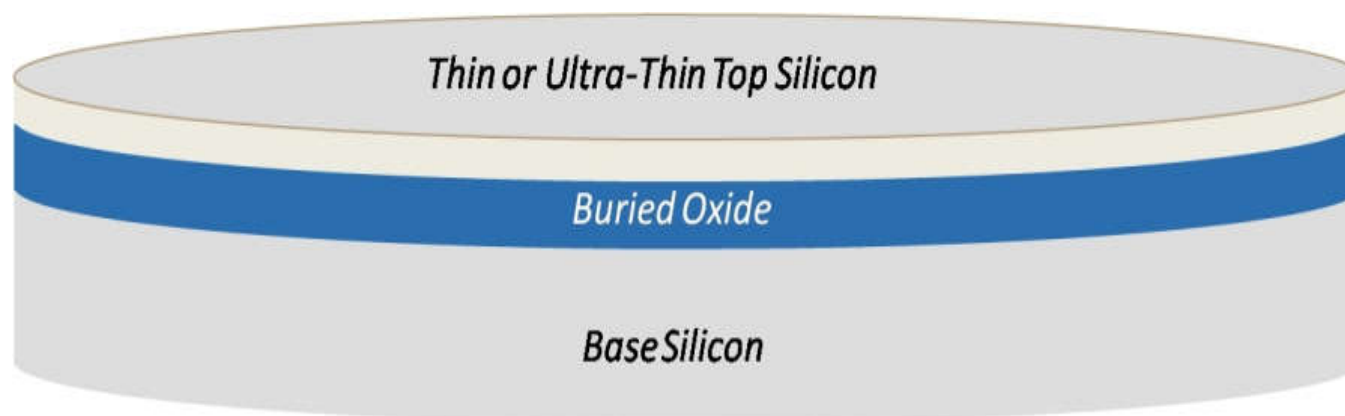
*why ???*

# Breaking Amorphous Materials

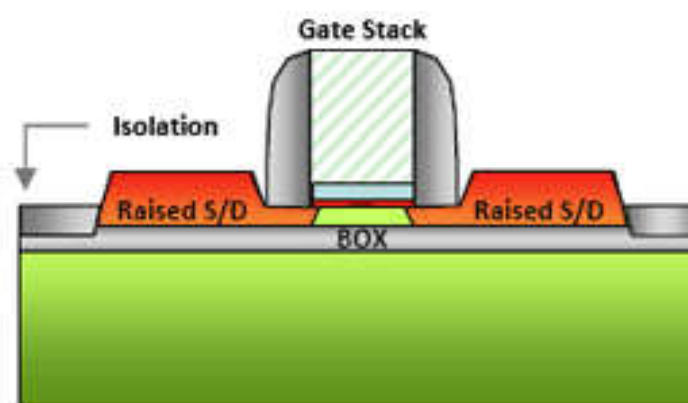


Amorphous

# Silicon-on-Insulator (SOI)

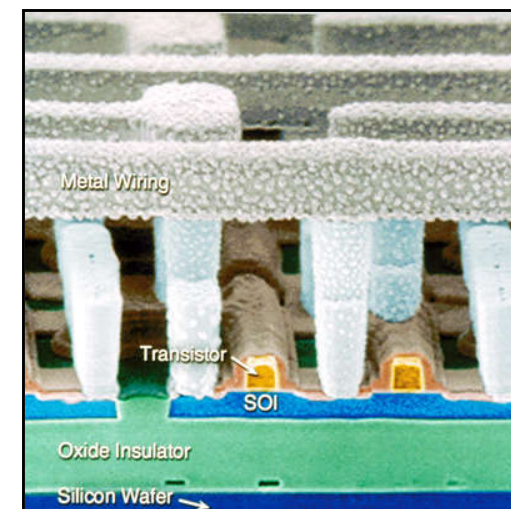


Bulk Device



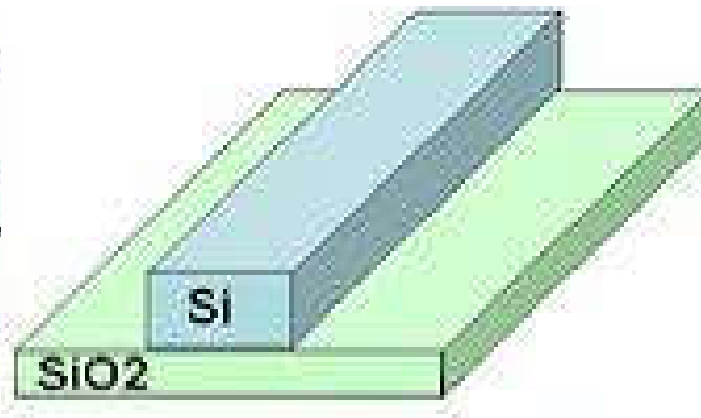
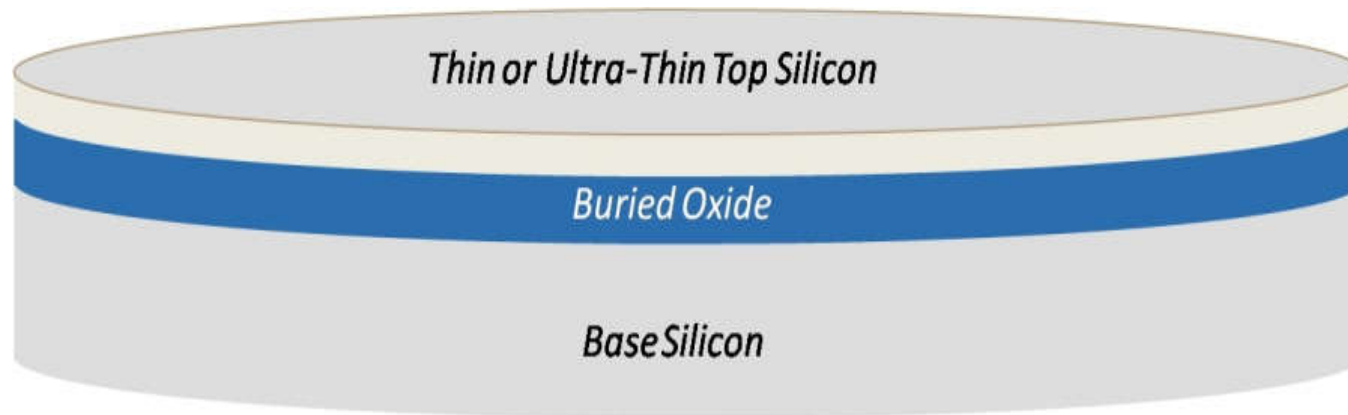
FD-SOI Device

The fully depleted SOI transistor at 20 nm is significantly simpler than even a simplified version of the bulk CMOS transistor.

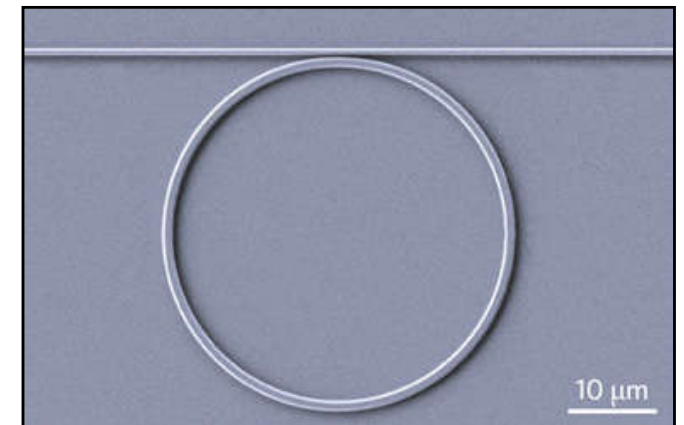




# Silicon-on-Insulator (SOI)



**Silicon waveguide**



**Ring resonator**



# Other single crystals



**Ge**



**GaAs**

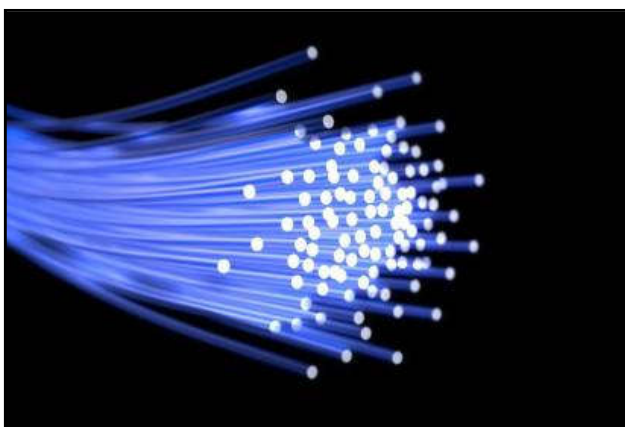


**sapphire**

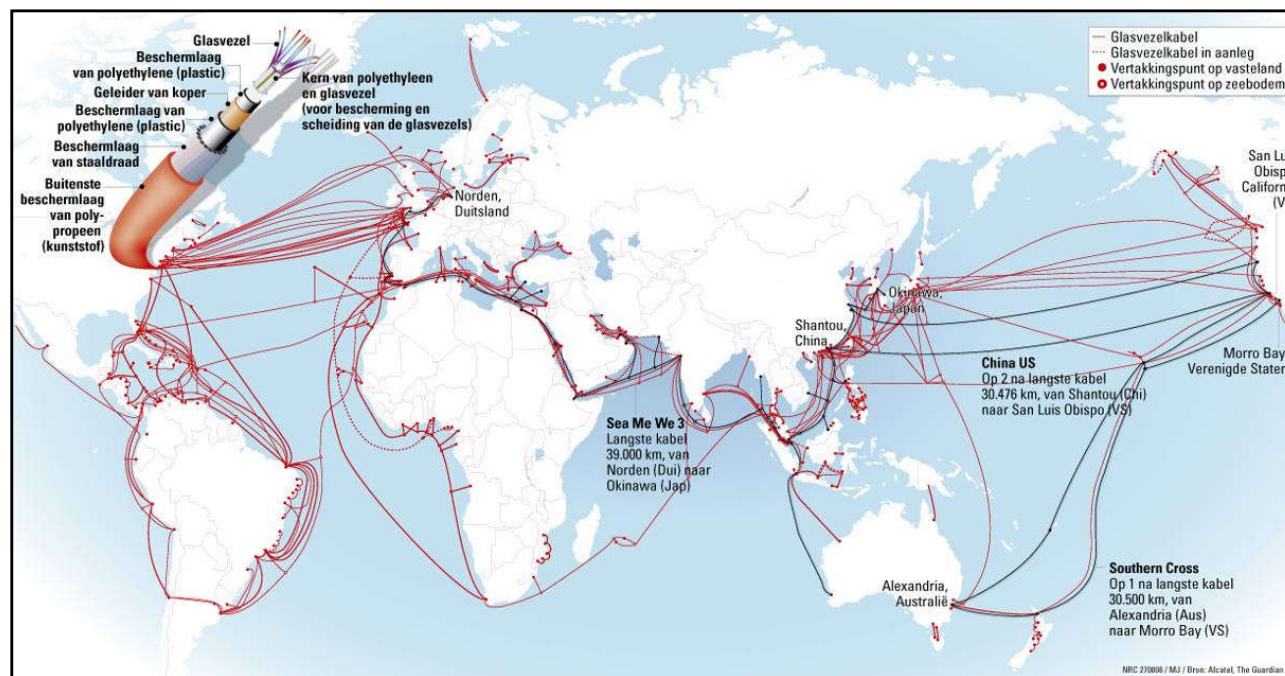


**Q: Can we make diamond crystals?**

# Optical Fibers



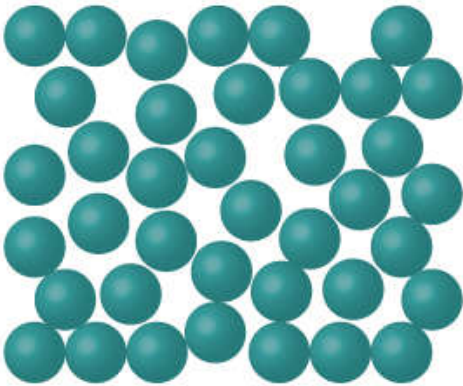
silica ( $\text{SiO}_2$ )



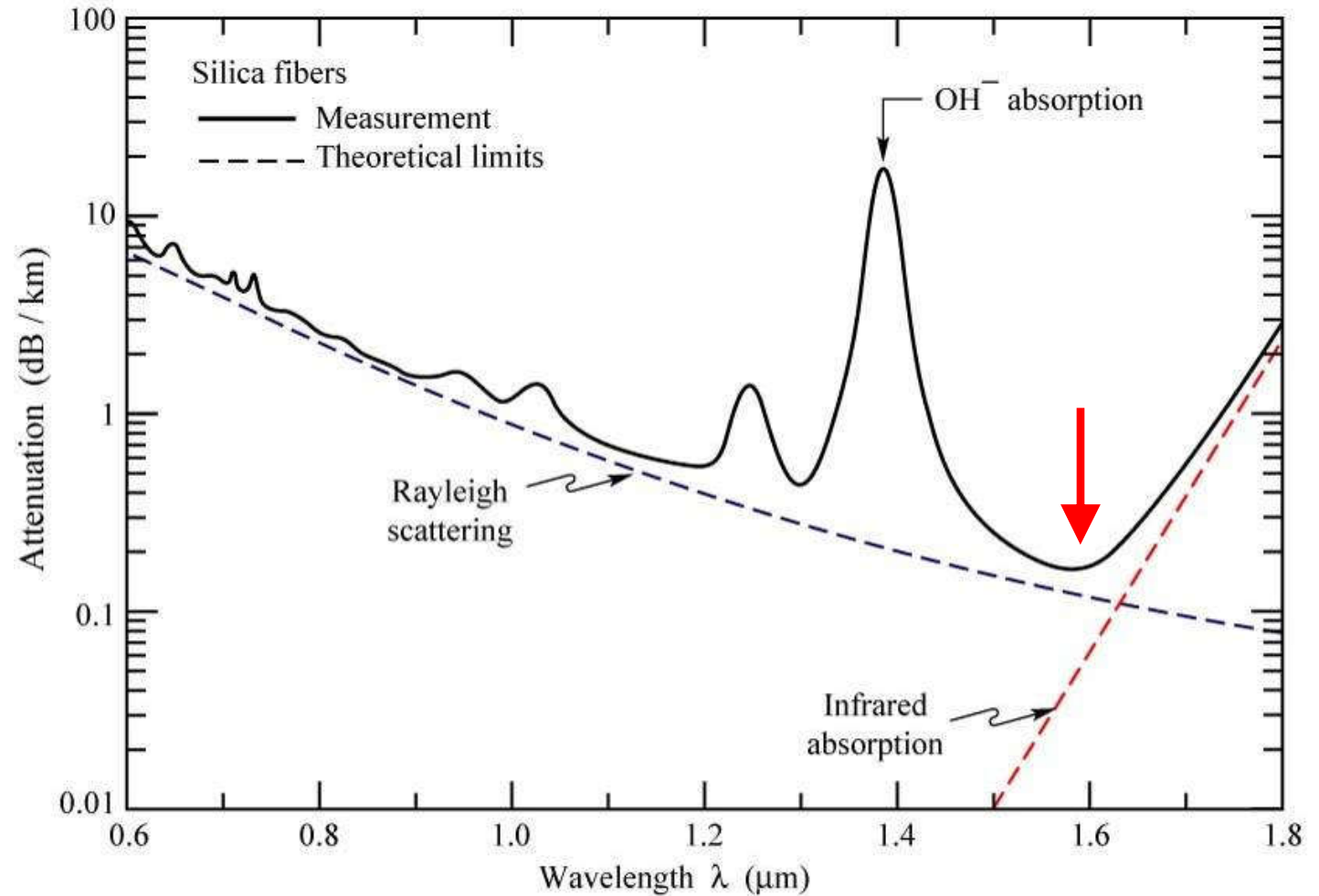
**K. Kao (高錕) (1933–2018)**  
**2009 Nobel Prize in Physics**

K. C. Kao, G. A. Hockham, *Proc. IEE* **113**, 1151 (1966)

# Absorption of Silica ( $\text{SiO}_2$ )



Amorphous



**minimum loss at 1550 nm, 0.2 dB/km**  
**~ 2% loss every kilometer**

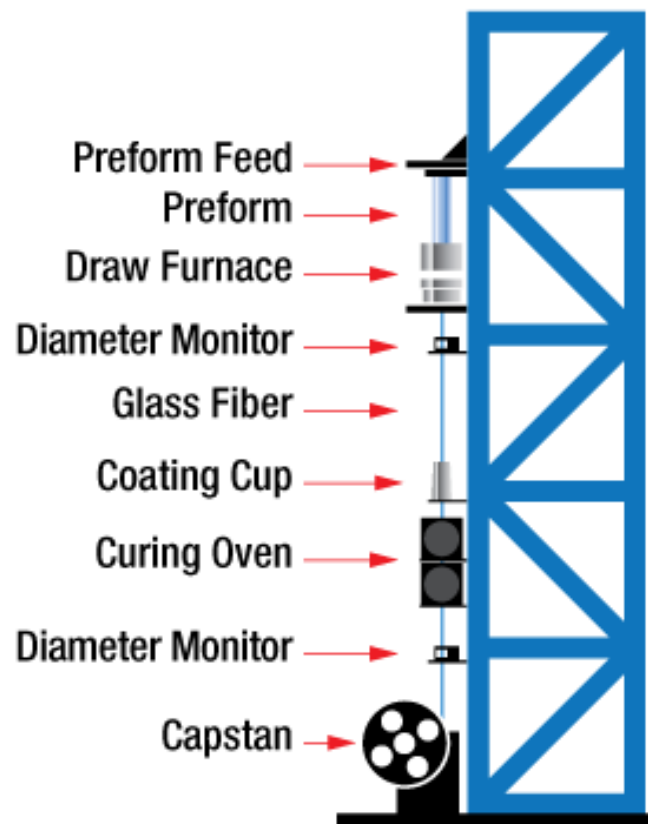
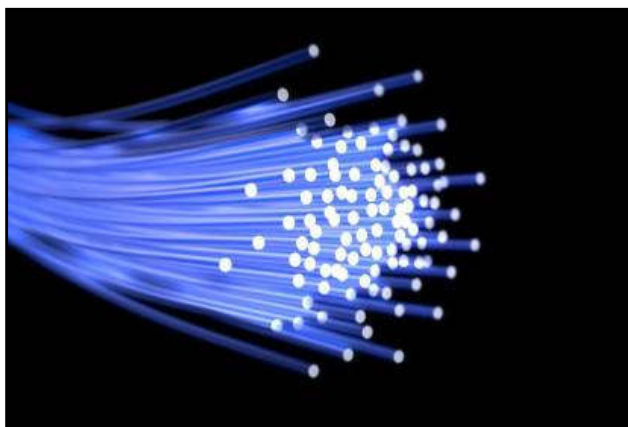


# Optical Fiber Drawing

preform



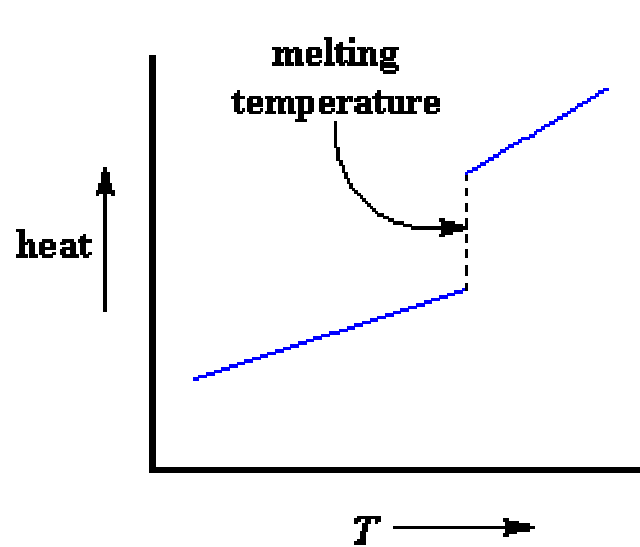
fibers



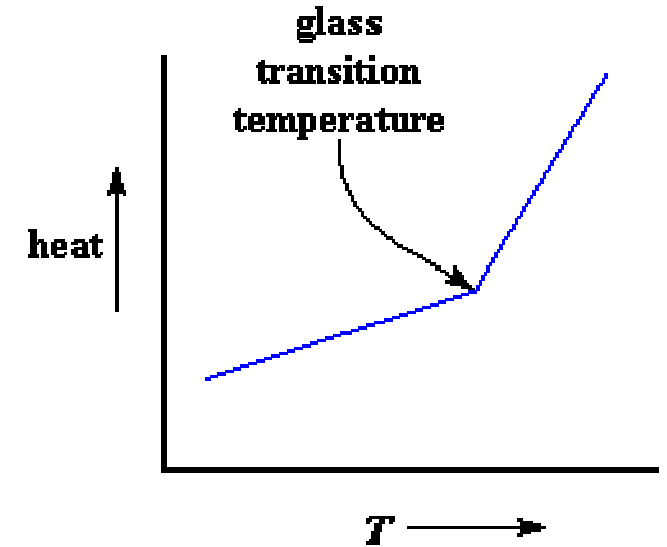
[Video](#)

# Glass Transition

## 吹玻璃



1st order transition



2nd order transition



glassy / plastic state



viscous / rubbery state



# Optical Fibers

